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Groundwater Modeling:

An Overview and Status Report

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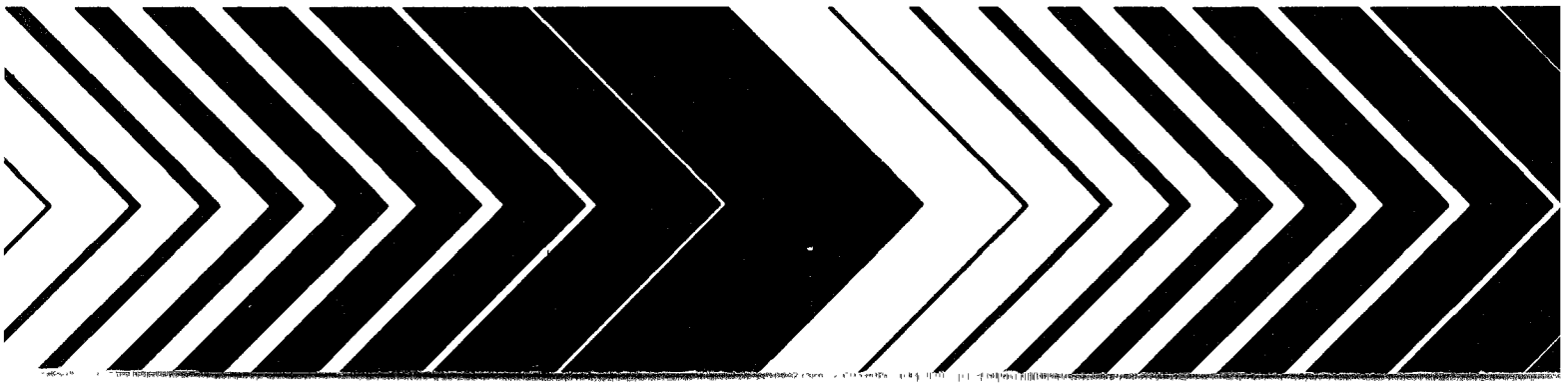

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December 1988

GROUNDWATER MODELING: AN OVERVIEW AND STATUS REPORT

by

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SUMMARY

This report focuses on groundwater models and their application in the management of water resource systems. It reviews the kinds of models that have been developed and their specific and general role in water resource management.

The report begins with the introduction of system concepts applicable to subsurface hydrology and presents groundwater modeling terminology, followed by a discussion of the role of modeling in groundwater management with special attention to the importance of spatial and temporal scales. The model development process is discussed together with related issues such as model validation. A separate section provides information on model application procedures and issues. In addition to a review of the model application process, this chapter contains discussion of model selection and model calibration and provides information on specific aspects of pollution modeling. The report also contains an extensive overview of current model status. Here, the availability of the models, their specific characteristics, and the information, data, and technical expertise needed for their operation and use are discussed. Also discussed are quality assurance in groundwater modeling and management issues and concerns. The report concludes with a review of current limitations in modeling and offers recommendations for improvements in models and modeling procedures.

FOREWORD

EPA is charged by Congress to protect the nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the Laboratory are responsible for management of research programs to: (a) determine the fate, transport and tranformation rates of pollutants in the soil, the unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and the subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil, and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to soil and subsurface environment, for the protection of this resource.

This report contains the result of a study performed to improve the quality of modeling in groundwater protection. It provides an introduction to groundwater modeling procedures and quality assurance, presents an overview of the status of major types of groundwater models, and discusses problems related to the development and use of groundwater models.

Clinton W. Hall
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BACKGROUND AND REPORT ORGANIZATION

In the mid-1970s, by request of the Scientific Committee on Problems of the Environment (SCORE), part of the International Council of Scientific Unions (ICSU), the Holcomb Research Institute (HRI) at Butler University, Indianapolis, Indiana, carried out a groundwater modeling assessment. This international study, funded in large part by the U.S. Environmental Protection Agency (EPA) through its R.S. Kerr Environmental Research Laboratory in Oklahoma, resulted in a report published by the American Geophysical Union (AGU) in its series, ***Water Resources Monographs***. In 1985 a second edition of this monograph (AGU Monograph 5) was published, based on information collected at HRI through its International Ground Water Modeling Center (IGWMC) from its inception in 1978 until December 1983. The Center was established at HRI as an international clearinghouse for groundwater models and a technology transfer center in groundwater modeling. Since 1983 the Center has been linked to the TNO Institute of Applied Geosciences, Delft, The Netherlands which operates the European office of the IGWMC. Supported largely by the EPA and in part by HRI, the Center operates a clearinghouse for groundwater modeling software, organizes and conducts short courses and seminars, and carries out a research program to advance the quality of modeling in groundwater management, in support of the Center's technology transfer functions. The Center's International Technical Advisory Committee provides guidance and active support to its program.

The present report contains the result of research and information processing activities performed by the IGWMC under a research and technology transfer cooperative agreement initiated in 1985. The report serves three functions: (1) it provides an introduction to groundwater modeling and related issues for use as instruction material in short courses and for self study; (2) it provides an overview of the status of major types of groundwater models; and (3) it presents a discussion of problems related to the development and use of groundwater models.

The review of models has been based on information gathered since 1975 by the Holcomb Research Institute, through research and interviews. To manage the rapidly growing amount of information, HRI, through its IGWMC, maintains a series of information databases, currently being transferred from the DEC/VAX environment to the 80286/80386 MS DOS environment.

The subject of this report is groundwater models and their application in the management of water resource systems. Attention is focused on the kinds of models that have been developed and their specific and general role in management. The availability of the models, their specific characteristics, and the information, data, and technical expertise needed for their operation and use are also discussed.

Chapter 1 introduces groundwater as a system accessible to analysis and simulation and presents the groundwater modeling terminology. In Chapter 2 the role of modeling in groundwater management is discussed with special attention to the importance of scale. Chapter 3 describes the model development process and discusses related issues such as model validation. In Chapter 4 model application, as it relates to environmental decision making, is discussed. In addition to a review of the model application process, this

chapter contains discussion of model selection and model calibration and provides information on specific aspects of pollution modeling. Chapter 5 overviews the current model status as an update of AGU Monograph 5 (second edition). Chapter 6 presents terminology and approaches to quality assurance in groundwater modeling, while Chapter 7 focuses on management issues and concerns. Finally, in Chapter 8 the authors discuss current limitations in modeling and offer recommendations for improvements in models and modeling procedures.

The authors are grateful to Milovan S. Beljin and P. Srinivasan for their past contributions to the IGWMC model assessment studies; to Richard E. Rice for his contributions on geochemical equilibrium models; to Deborah L. Cave for her assistance in collecting model information and reviewing hydrochemical modeling literature; to Michal Stibitz for his assistance in processing model information; to Margaret A. Butorac and Karen Ochsenrider for project assistance; to Ginger Williams and Eric Roach for word processing; to James N. Rogers for manuscript editing; and to Colleen Baker and Barbara Stackhouse for graphics.

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1. INTRODUCTION

Groundwater modeling is a methodology for the analysis of mechanisms and controls of groundwater systems and for the evaluation of policies, actions, and designs that may affect such systems.

Models are useful tools for understanding the mechanisms of groundwater systems and the processes that influence their composition. Modeling serves as a means to ensure orderly interpretation of the data describing a groundwater system, and to ensure that this interpretation is a consistent representation of the system. It can also provide a quantitative indicator for resource evaluation where financial resources for additional field data collection are limited. Finally, models can be used in what is often called the predictive mode by analyzing the response a system is expected to show when existing stresses vary and new ones are introduced: they can assist in screening alternative policies, in optimizing engineering designs, and in assessing operative actions in order to determine their impacts on the groundwater system and ultimately on the risks of these actions to human health and the environment.

In managing water resources to meet long-term human and environmental needs, groundwater models have become important tools.

The field of groundwater modeling is expanding and evolving as a result of:

- Widespread detection of contaminated groundwater systems
- Enhanced scientific capability in modeling groundwater contamination in terms of the physical, biological, and chemical processes involved
- Rapid advancement of computer software and hardware, and the marked reduction in the cost associated with this technology.

The rapid growth in the use of groundwater models has led to unforeseen problems in project management. Some of the projects in which these sophisticated tools have been used have even led to adversary legal procedures in which the model application or even the model's theoretical framework and coding have been contested. Often, the key issue is the validity of model-based predictions. Other issues of concern include code availability and reliability, model selection and acceptance criteria, project review and procurement, data requirements, information exchange, and training.

THE GROUNDWATER SYSTEM

Groundwater is a subsurface element of the hydrosphere, which is generally understood to encompass all the waters beneath, on, and above the earth's surface. Many solar-powered processes occur in the hydrosphere, resulting in a continuous movement of water. This dynamic system is referred to as the hydrologic cycle. Its major elements are atmospheric water, surface water, water in the subsoil (shallow and deep vadose zone), groundwater, streams, lakes and ocean basins, and the water in the lithosphere (Figure 1).

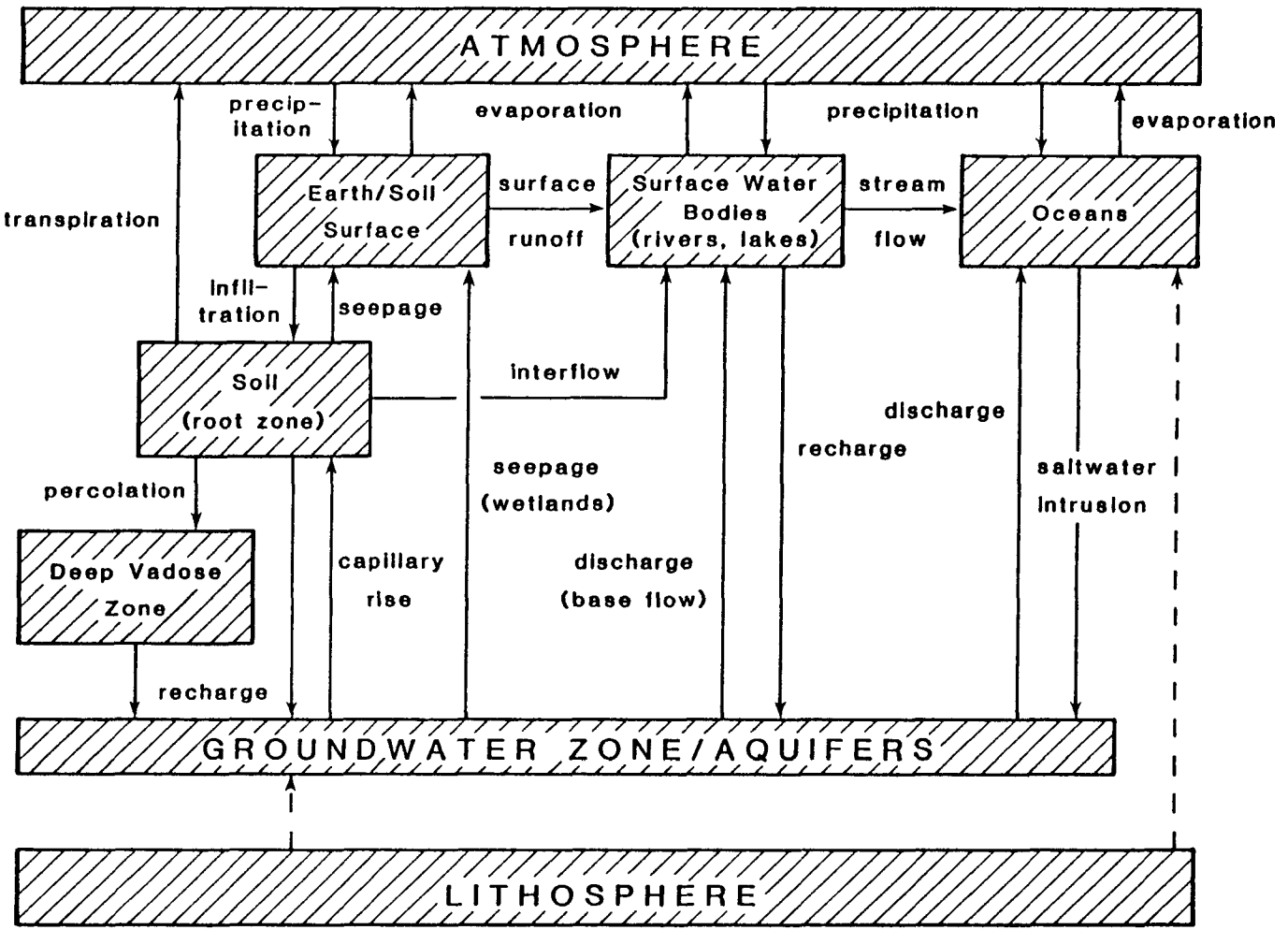


Fig. 1. Elements of the hydrologic cycle and their interactions.

Movement of water occurs both within each element of the hydrologic cycle and as exchanges between the elements, and results in the dynamic character of this relatively closed system. The exchange processes between the surface subsystem and the atmosphere include evaporation, precipitation (rainfall and snowfall), and plant transpiration. Infiltration, seepage, groundwater recharge from streams, and subsurface discharge into lakes and streams (both interflow and baseflow) are inter-element processes between the earth's surface and subsurface. Surface runoff forms the link between the earth's surface and the network of streams. In addition, interactions take place between the subsurface hydrosphere and elements of the earth's biological environment (e.g., consumptive use of water by plants).

A groundwater system is an aggregate of rock in which water enters and moves, and which is bounded by rock that does not allow any water movement, and by zones of interaction with the earth's surface and with surface water systems (Domenico 1972). In such a system the water may transport solutes and biota; interactions of both water and dissolved constituents with the solid phase (rock) often occur.

Water enters the groundwater system in recharge zones and leaves the system in discharge areas. In a humid climate, the major source of aquifer recharge is the infiltration of water and its subsequent percolation through the soil into the groundwater subsystem. This type of recharge occurs in all in-stream areas except along streams and their adjoining floodplains, which are generally discharge areas. In arid parts of the world, recharge is often restricted to mountain ranges, to alluvial fans bordering these mountain ranges, and along the channels of major streams underlain by thick and permeable alluvial deposits.

In addition to these natural recharge processes, artificial or man-made recharge can be significant. This type of recharge includes injection wells, induced infiltration from surface water bodies, and irrigation.

Outflows from groundwater systems are normally the result of a combination of inflows from various recharge sources. Groundwater loss appears as interflow to streams (rapid near-surface runoff); as groundwater discharge into streams (resulting in stream baseflow); as springs and small seeps in hillsides and valley bottoms; as wetlands such as lakes and marshes fed by groundwater; as capillary rise near the water table into a zone from which evaporation and transpiration can occur; and as transpiration by phreatophytes (plants whose roots can live in the saturated zone or can survive fluctuations of the water table) (Toth 1971, Freeze and Cherry 1979). Other outflows are artificial or human-induced, as agricultural drainage (tile-drains, furrows, ditches) and wells for water supply or dewatering (e.g., excavations and mining).

The unsaturated zone has a significant smoothing influence on the temporal characteristics of the recharge of groundwater systems. Highly variable (hourly) precipitation and diurnal evapotranspiration effects are dampened and seasonal and long-term variations in flow rates become more prominent further from the soil surface. In this dampening the higher-frequency fluctuations are filtered, a process that continues in the groundwater zone. Its ultimate effect can be observed in stream base flow, which is characterized by seasonal and long-term components.

A groundwater system may consist of a single flow system between its recharge and discharge areas. This is generally the case when local relief is negligible and only a gentle regional slope is present. If the relief of the surface becomes more pronounced, local groundwater flow systems can develop. If the depth-to-length ratio of the system in the direction of principal surface gradients is small, a series of local flow systems adjacent to each other is the result. However, if the aquifer depth-to-width ratio increases, a combination of flow systems may develop, resulting in a hierarchically structured groundwater system with local, intermediate, and regional components (Figure 2) (Toth 1963). If the groundwater system consists of multiple aquifers, this hierarchical structure is even more evident (van der Heijde 1988) (Figure 3). The notion that such a hierarchical structure exists has improved the effectiveness of modeling groundwater systems significantly (e.g., Freeze and Witherspoon 1966).

The largest hydrogeologic unit is a groundwater basin. It is a system containing the entire network of flow paths taken by all the water recharging the basin (Freeze and Witherspoon 1966). A groundwater basin consists of a single aquifer or several connected and inter-related aquifers. The water divide between two adjacent groundwater basins is not necessarily the same as that between the surface water drainage basins overlying them. Watersheds can lose part of their water to neighboring watersheds through subsurface inter-basin transfers. In a valley between mountain ranges, the drainage basin of the surface stream coincides closely with the groundwater basin. In limestone areas and large alluvial basins, the drainage and groundwater basins may have entirely different configurations.

A groundwater system has two basic hydraulic functions: it is a reservoir for water storage, and it serves as a conduit by facilitating the transmission of water from recharge to discharge areas. A groundwater system can be considered as a reservoir that integrates various inputs and dampens and delays the propagation of responses to those inputs (van der Heijde 1988). The water movement is dictated by hydraulic gradients and system-dependent hydraulic conductivity. In turn, these gradients are influenced by boundary conditions on the groundwater system. These conditions could include anthropogenic stresses on the system (e.g., pumping), climatic effects, surface topography, and other possible geomorphic features of the physical system such as streams, reservoirs, etc.

The rate of groundwater movement can be expressed in terms of time required for groundwater to move from a recharge area to a discharge zone. This time ranges from a few days in zones adjacent to discharge areas in small local systems, to thousands of years for water that moves through deeper parts of the groundwater system (Figure 3).

Groundwater systems are characterized by complex relationships among patterns for system recharge, discharge, and groundwater storage. Obviously, system discharge patterns are influenced by the origin and pathways of the groundwater. For several reasons, the relationships are difficult to define directly from observed input and response data. These include the dampening effect of storage on inflow, the lag or delay between the time water enters and exits the system, the variable rate and sometimes diffuse nature of recharge and discharge, and the heterogeneous nature of the geologic system. Therefore, deterministic, mathematical models, based on a mechanistic descrip-

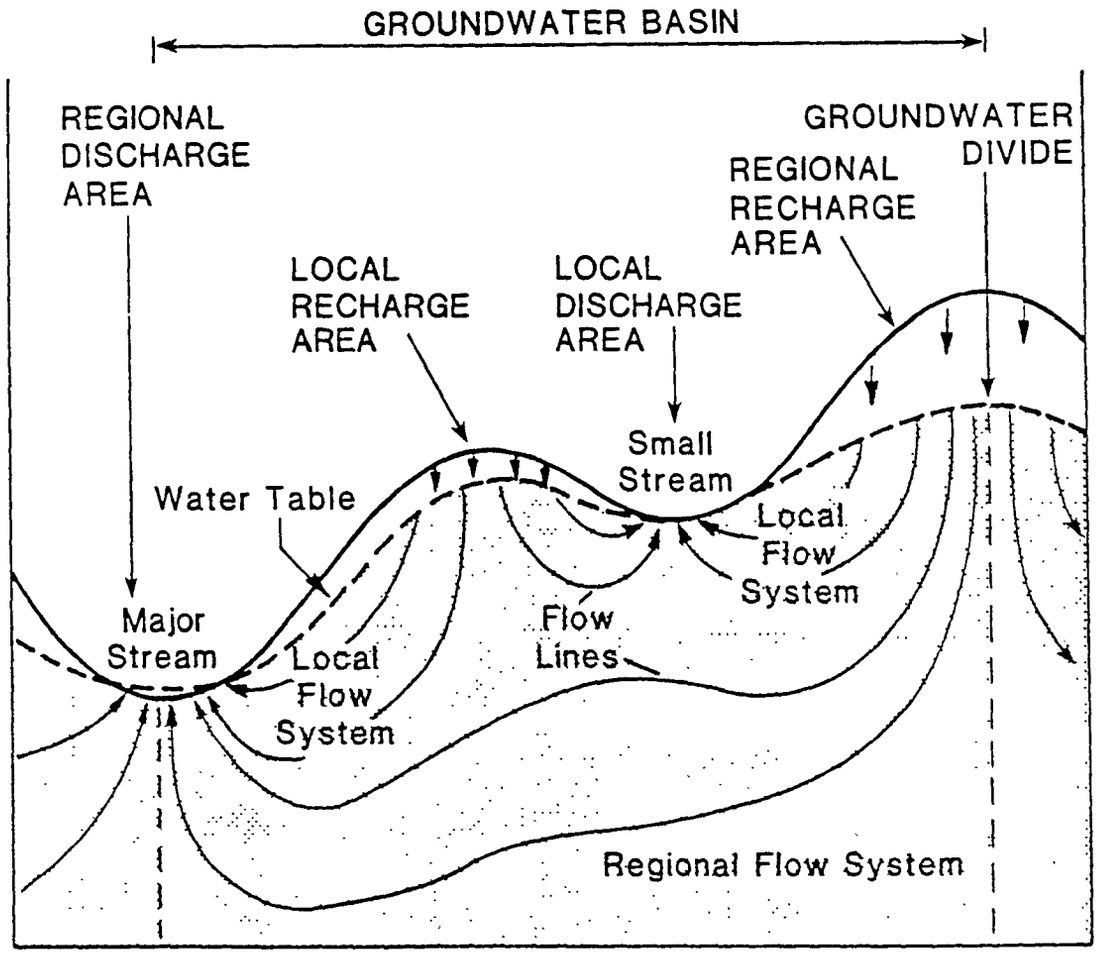


Fig. 2. Schematic diagram of a regional groundwater system (after Toth 1963).

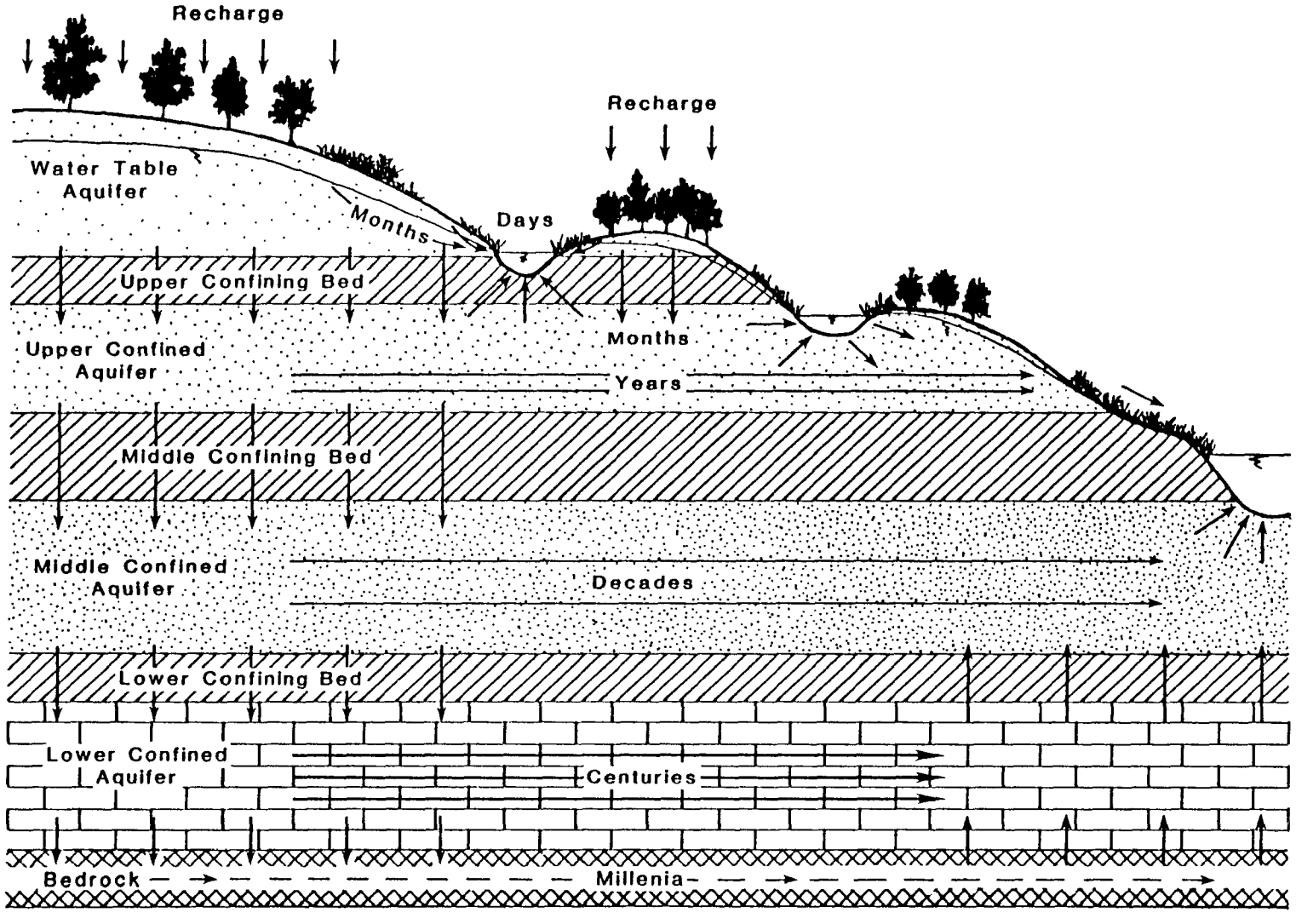


Fig. 3. Schematic overview of groundwater resident times in large regional systems (after van der Heijde 1988).

tion of the physical and chemical processes that describe the groundwater system, are widely used in groundwater hydrology (van der Heijde 1988).

GROUNDWATER QUALITY

In the last few decades, groundwater contamination from organic and inorganic chemicals, radionuclides, and microorganisms from domestic, industrial, and agricultural activities has become a significant environmental problem (EPA 1977, Jackson 1980, Pye et al. 1983, NRC 1984). This increased concern with the quality of groundwater has been catalyzed by the widespread detection of contamination of groundwater systems, more public awareness of the health and environmental risks associated with groundwater contamination, and the increase of industrial waste and the problem of hazardous waste disposal (OTA 1984).

The quality of groundwater is typically described by its chemical composition. This quality is the result of natural processes and human intervention, either by introducing chemical or biological components directly into the groundwater system, or indirectly by modifying the effects of natural processes on the system (e.g., salt water intrusion).

Natural groundwater can be defined as groundwater whose composition is determined only by natural, non-human-induced processes. The composition of natural groundwater is the result of its hydrogeological and geochemical history. In its role as part of the hydrologic cycle, groundwater is recharged by water from the atmosphere and from bodies of surface water. It is now or once was part of a dynamic system of movement through and interaction with the geologic environment.

Atmospheric precipitation, because of its chemical composition and physical characteristics, is a major influence on the quality of groundwater. It is a source of such chemicals as oxygen, nitrogen, and carbon dioxide and is slightly acid (pH $\approx$ 6.5; Hem 1970). This acidity can increase significantly (e.g., pH 2-4) when man-made pollutants such as oxides of sulfur and nitrogen are introduced into the atmosphere.

Precipitation can have a diluting effect on groundwater, as when the concentration of dissolved chemicals in the precipitation is lower than that of the groundwater. In addition, the precipitation temperature can alter the temperature of the soil and thus change reaction and transformation rates of groundwater processes in the soil.

Another important natural process is evaporation, which can influence the amount of water available for infiltration to deeper formations, thus reducing the diluting effect of precipitation on groundwater. Evaporation can have a concentrating effect on salts in soil; only the water evaporates and the solutes are left behind.

Infiltrated water is a potential leaching agent of soils and rock. In arid regions, leaching is a major cause of saline pollution of groundwater, resulting in a high value for total dissolved solids and high chloride content of the groundwater. Other common natural leachate products are sulfates, nitrates, fluorides, and iron (Hem 1970). Under the influence of the carbon

dioxide introduced into the soil and hence into groundwater, calcium and magnesium carbonate are formed, resulting in an increase in water hardness. In some areas leaching of uranium ore under natural conditions causes a significant increase in the natural radioactivity of soil.

Sources of Groundwater Pollution

Although human intervention in the environment began many centuries ago, its significant effects on groundwater are of recent origin, and in general are restricted to regions of significantly altered land use, as by urbanization, mining, or agriculture.

Pollution of groundwater may result from direct introduction of chemical or biological components, and indirectly from induced alterations in water quality through modification of external or related system conditions. Such intervention may be the result of planned or illegal domestic, commercial, industrial, or agricultural waste disposal; upconing of saline water by pumping a freshwater aquifer over a saltwater aquifer; discharge of polluted water in streams that recharge aquifers; mine drainage; acidification of soils by acidic precipitation resulting from industrial and vehicular releases of contaminants; runoff from road deicing salts; infiltration of polluted surface water; and by salt water intrusion from oceans or from saline aquifers. The intervention may also be accidental, as with spills and leakage of storage tanks and pipelines.

A major cause of widespread groundwater pollution is the introduction of solid and liquid wastes into the subsurface or near-surface soil. Liquid waste and the leachate from solid waste directly affect groundwater quality. The resulting deterioration in water quality may be so serious that the source is a hazard to human health or the environment.

Various types of solid wastes occur: domestic waste, solid commercial waste, solid compounds of industrial waste, sludge from waste treatment plants, sludge from water supply treatment plants or air-pollution control facilities, and mine tailings. As determined by the type of waste, various leachate compositions may develop. For example, the leachate of household waste contains high concentrations of sulfate, chloride, and ammonia. Commercial solid waste produces oils, phenols, and organic solvents. A more complete description of the composition of various waste leachates is presented by Jackson (1980) and Pye et al. (1983).

Solid waste is often disposed of through dumps, landfills, sanitary landfills, or secured landfills. Uncontrolled dumps and weakly controlled landfills are the major causes of groundwater pollution. The leachate formed from these sources consists primarily of dissolved minerals, heavy metals, and organic chemicals.

Another major source of groundwater pollution is liquid waste. Various disposal methods are in use, such as wastewater impoundments, deep subsurface injection, land spreading of the liquid waste, and discharge into surface water bodies. The waste water may be diluted before it is discarded.

A major type of liquid waste is municipal wastewater, which consists of domestic, industrial, and stormwater components. Although municipal waste-

water is often treated before it is discharged into the environment, many sanitary sewer systems leak untreated wastewater into the ground. This is particularly true when sewer pipes are above the water table and water pressure is not available to prevent leakage of the sewage. If the sewer system is also used for stormwater removal, heavy storms can cause overflow of the storage lagoons in the system, thus contributing to groundwater pollution by direct infiltration into the soil. Finally, land disposal of treated municipal wastewater may cause problems. Various disposal methods are used, such as agricultural irrigation, rapid infiltration ponds, overland runoff, discharge into dry streambeds and ditches, and land spraying.

Industrial wastewater is often disposed of directly by the industry that produces it. Treated wastewater may be discharged to a surface water body. Untreated wastewater is often stored in impoundments such as pits, ponds, lagoons, or pools, either temporarily until treatment is available, or indefinitely. Leakage of wastewater into the ground occurs frequently with this type of waste storage. The leakage may be caused by a poorly designed or constructed facility, such as one without liners or with leaking liners, or by accidental overflow of basins resulting in infiltration into the underlying soil. Some impoundments are designed to overflow and discharge regularly into bays, oceans, lakes, or streams. Liquid waste in nondischarging impoundments may be lost through evapotranspiration or seepage into the soil. The liquid residuals of oil and gas extraction and animal feedlot wastes are often stored in such impoundments.

Another method of liquid waste disposal is through deep well injection. This method, which is frequently used to dispose of brine and other residuals from oil and gas drilling and well-bore maintenance, is also used for various industrial wastes. Major problems with this method are leakage through the well bore because of construction faults, or breakthrough and seepage through the confining layers separating an aquifer targeted for disposal from an aquifer utilized for water supply. Such breakthrough and seepage may result from insufficient thickness of the confining layer or from hydraulic fracturing. In certain areas, hydraulic short circuiting through abandoned oil and gas wells occurs. Problems arising from with deep well injection often are caused by the high pressures necessary to force the waste into the aquifer. Direct injection into an already-exploited aquifer may occur, or the increased pressures caused by the injection may cause displacements of saline waters toward water supply wells. In some cases the injected waste migrates to a freshwater part of the aquifer and causes deterioration of its quality.

Widespread use of individual sewage disposal systems is another major wastewater source discharging directly into groundwater. Three methods of on-site domestic waste disposal are practiced: septic tanks with a subsurface disposal system, cesspools, and pit privies. All three are located in the near-surface soil. Properly sited, constructed, and maintained septic tanks are generally no problem. However, many septic tanks are not well-constructed or are poorly maintained and overloaded (Pye et al. 1983).

Accidental spills and leakage form another category of liquid waste pollution sources. These can occur in a wide variety of situations, as in industrial processes, storage activities, and during transport. In general, the effects of these pollution sources are local, although their ultimate effects on groundwater quality may be wide-ranging.

The major causes of pollution from agricultural activities are the widespread use of pesticides, herbicides, and fertilizers, and the production of manure, especially in feedlots. Application of fertilizers to crops often leads to nonpoint pollution from runoff organics and nitrate. Irrigation return flow can contribute significantly to this problem.

A special type of pollution is caused by radioactive waste disposal. Frequently, this waste contains solid, liquid, or gaseous chemicals of both radiological and chemical toxicity. From a management point of view, two types of radioactive waste are distinguished: high and low level. In general, these are disposed of in a controlled manner. However, transport spills and accidental operational discharges to the environment may occur. Identification of the source, its chemical characteristics and its temporal behavior are important issues in studying groundwater pollution problems. Knowing source location and behavior is prerequisite to most groundwater modeling efforts. It influences model selection and modeling strategy and ultimately the accuracy of model-based predictions.

A more detailed discussion of modeling groundwater quality is presented in Chapter 4.

GROUNDWATER MODELING: DEFINITIONS

Although a consensus may exist as to what groundwater modeling entails, the definition of a "model" per se is somewhat nebulous. As a generalized definition, a model is a non-unique simplified description of an existing physical system. In order to create such a simplified version of the system, various assumptions are made with respect to physical system characteristics, technical issues involved, and relevant managerial constraints. Groundwater models are generally intended to provide practical, descriptive, and predictive problem-solving tools.

Although physical groundwater models can be useful for studying certain problems, the present focus is on mathematical models in which the causal relationships among various components of the system and the system and its environment are quantified and expressed in terms of mathematics and uncertainty of information. This definition is still rather broad and is not limited to where the physical, chemical and biological processes themselves are well defined. Thus, mathematical models might range from rather simple, empirical expressions to complex multi-equation formulations.

In hydrogeology, the term "groundwater model" has also become synonymous with conceptual models, mathematical models, analytic or numerical models, computer models, and simulation models. (A detailed discussion of these latter terms is given in Chapter 5.) For the present discussion of computer-based modeling, we refer to a groundwater model as the mathematical description of the processes active in a groundwater system, coded in a programming language, together with a quantification of the groundwater system it simulates in the form of boundary conditions and parameters. The generic computer code that is used in this problem-specific system simulation is often referred to as a computer model. The most complex of these simulation models are usually based on numerical solution techniques which allow simulation of heterogeneous systems controlled by a variety of coupled processes that des-

cribe the hydrology, chemical transport, geochemistry, and biochemistry of the heterogeneous near-surface and deep underground. This use of the term groundwater model includes fluid flow and solute transport models for both the saturated and unsaturated zones and reflects the highly multidisciplinary nature of contemporary hydrogeology. Although other types of models have been developed for simulating soil processes and processes in the deeper subsurface (e.g., air and vapor transport in soils, soil mechanics, fracture propagation, stress-strain behavior of rock, and steam flow and related heat transport in multiphase geothermal reservoirs, the discussion in this report is restricted to models that relate directly to soil and groundwater.

2. GROUNDWATER MODELING AND MANAGEMENT

Groundwater management is concerned with the efficient utilization of groundwater resources in response to current and future demands, while protecting the integrity of the resources to sustain general environmental needs. Groundwater modeling has become an important methodology in support of the planning and decision-making processes involved in groundwater management.

Groundwater modeling provides an analytical framework for understanding groundwater flow systems and the processes and controls that influence their quality, particularly those processes influenced by human intervention in the hydrogeologic system. Models can provide water resource managers with necessary support for planning and screening of alternative policies, making management decisions, and reviewing technical designs for groundwater remediation based on a risk analysis of benefits and costs. Such support is particularly advantageous when applied to development of groundwater supply, groundwater protection, and aquifer restoration.

Successful utilization of modeling is possible only if the methodology is properly integrated with data collection, data processing, and other techniques and approaches for evaluation of hydrogeologic system characteristics. Furthermore, frequent communication between managers and technical experts is essential to assure that management issues are adequately formulated and that the technical analysis using models is well targeted.

GROUNDWATER RESOURCE DEVELOPMENT

According to Freeze and Back (1983), the earliest application of numerical simulation to a subsurface flow problem was documented in Shaw and Southwell (1941). In those days all calculations were performed by hand. Stallman (1956) is considered the first to have shown the feasibility of applying numerical methods in groundwater hydrology. In the 1960s, the rapid development of computer technology made it possible to simulate groundwater systems efficiently through the use of software instead of physical scale models or electric analogs. Since that time, modeling has become an increasingly popular and useful tool in groundwater management (Prickett 1975).

Since the major means to exploit groundwater resources is through pumping, management is concerned with determining location, spacing, and sizing of wells or well fields, and the rates and time schedules of pumpage. Extracting groundwater through pumping might reduce the natural discharge of groundwater in streams and thus reduce base flow. In addition, if the pumping is excessive enough to lower the water levels significantly, exploitation of the resource may lead to land subsidence or, in karstic areas, to collapse of the ground surface.

With the development of computer technology and modeling methodology, more powerful tools became available for investigations into such groundwater management issues as the optimum design of well fields, the quantitative analysis of regional groundwater supplies, and the prediction of water level declines due to groundwater withdrawals. The first groundwater computer models were constructed to facilitate the development of well fields in local

and regional aquifer systems while limiting the environmental impacts of such developments.

From the beginning, the U.S. Geological Survey (USGS) has contributed significantly to groundwater modeling. In the late 1960s the USGS initiated the development of digital models to replace analog models (Pinder and Bredehoeft 1968). Since then, the USGS has developed a comprehensive suite of generic simulation and parameter estimation models, many of which are widely used in the United States and abroad. An overview of the early USGS contributions to groundwater modeling was presented by Appel and Bredehoeft (1976). Recently, Appel and Reilly (1988) compiled a listing of all pertinent USGS modeling codes.

GROUNDWATER QUALITY

The predictive capabilities of groundwater quality models are used to evaluate the potential impact of design alternatives for waste disposal facilities, proposed alterations in the groundwater flow system either through changing its boundaries, parameter values, or stresses (e.g., development of well fields, excavations for construction sites or open-pit mining, and dewatering operations), and the development of aquifer protection zones.

Where precise aquifer and contaminant characteristics have been reasonably well established, groundwater models may provide a viable, if not the only, method to predict contaminant transport and fate, locate areas of potential environmental risk, identify pollution sources, and assess possible remedial actions. Some examples in which mathematical models have assisted in the management of groundwater protection programs are (van der Heijde and Park 1986):

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

Models generally applied to groundwater pollution problems can be divided in two broad categories: (1) flow models describing hydraulic behavior of single or multiple fluids or fluid phases in porous soils, or porous or frac-

tured rock, and (2) contaminant transport and fate models for analysis of movement, transformation, and degradation of chemicals present in the subsurface. In the context of groundwater protection programs a distinction is often made between site-specific and generic modeling.

The success of a given model depends on the accuracy and efficiency with which the natural processes controlling the behavior of groundwater, and the chemical and biological species it transports, are simulated. The accuracy and efficiency of the simulation, in turn, depend heavily on the applicability of the assumptions and simplifications adopted in the model, the availability and accuracy of process information and site characterization data, and on subjective judgments made by the modeler and management.

It should be noted that the dimensionality required for solving the pollution problem adequately must be matched by the dimensionality of the model. One- and two-dimensional characterizations of the subsurface are no longer widely accepted for such analysis, as is illustrated by the rapid increase in applications of quasi- and fully three-dimensional models. Actual flow and transport in the three-dimensional environment can differ markedly from predictions obtained from one- and two-dimensional models based on idealizations of the three-dimensional world, even if the aquifer properties do not change significantly with depth.

Site-Specific Modeling

Whether for permit issuance, investigation of potential problems, or remediation of proven contamination, site-specific modeling is required as a necessary instrument for compliance under a number of major environmental statutes. The National Environmental Policy Act of 1970 (NEPA) stipulates a need to show the impact of major site-specific construction activities in Environmental Impact Statements; although not required by the regulations, potential impacts are often projected successfully by mathematical models.

Some of the most challenging site-specific problems involve hazardous waste sites falling under the purviews of RCRA (Resource Conservation and Recovery Act of 1976) and CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act of 1980—Superfund), both administered by the U.S. Environmental Protection Agency. Associated with most of these sites is an intricate array of chemical wastes and the presence of or potential for groundwater contamination. Furthermore, the hydrogeologic settings of such sites are usually complex. Under such conditions, groundwater models are useful instruments for analyzing compliance with RCRA and CERCLA legislation.

Generic Modeling

Where the results of environmental analysis must be applied to many sites, data availability is limited or other constraints are present. In such cases, site-specific modeling is not feasible. As a result, many decisions are made by applying models to generic management issues and hydrogeologic conditions. Models used for this type of analysis are more often analytical than numerical in their mathematical solutions, in contrast to models used for detailed analysis of site-specific conditions. Because of their limited data requirements, analytical models can be applied efficiently to a large number of simple datasets or to statistical analyses representing a wide variety of

field conditions. The cost of such exercises would often be prohibitive when using numerical models. However, the limitations imposed by analytical models on the simulation of a complex groundwater system require restraint in the use of computed results. Therefore, in choosing representative scenarios and model input, a so-called "conservative" approach is frequently taken, thus lowering the risk for subsequent management decisions.

Typical examples of generic modeling reflect the statutory responsibilities of such agencies as the U.S. EPA (van der Heijde and Park 1986), including the estimation of potential environmental exposures and their integration with dose-response models to yield health-based risk assessments. These assessments are necessary, for example, in issuing compound-specific rulings on products subject to preregistration requirements under the Toxic Substances Control Act of 1976 (TSCA) and the Federal Insecticide, Fungicide, and Rodenticide Act of (FIFRA). More generalized policy formulations also benefit from generic modeling; examples include policy decisions about land disposal "banning," setting Alternate Concentration Limits (ACLs), preparing Technical Enforcement Guidance Documents (i.e., for monitoring network designs), and "delisting" of particular types of waste under RCRA.

However, generic modeling approaches are being increasingly contested through public comment on draft regulations or in courtroom legal procedures. An example is the recent court decision that EPA's VHS model (Vertical Horizontal Spread model, EPA 1985) cannot be used to grant or deny a delisting petition under the RCRA permitting program (*Ground Water Monitor*, February 17, 1988, p. 26). Another example is the shelving of the EPA Screening Level Model (SLM) designed for use in the development of banning decisions regarding land disposal under RCRA, as a result of changes in interpretation of EPA's mandate in this area (EPA 1986a).

SCALES RELEVANT TO GROUNDWATER MANAGEMENT

A major aspect of the application of models is defining the spatial and temporal scales to be used in the model. Different scales might apply to various subsystems simulated by the model. The selection of scales is dependent on the management of objectives, the nature of the system(s) modeled, and the chosen numerical method, among other considerations.

A wide range of both spatial and temporal scales is involved in the study of groundwater problems. Spatial scales range from less than a nanometer, for studying such phenomena as the interactions between water molecules and dissolved chemicals (Cusham 1985), to hundreds of kilometers, for the assessment and management of regional groundwater systems (Toth 1963). For temporal scales, two major categories can be distinguished: steady-state or average state, and a time-varying or transient state. Periodic fluctuations on a diurnal or seasonal scale are frequent in hydrogeology. Other processes display certain trends or occur rather randomly in nature (Table 1). Many processes exhibit a strong temporal effect immediately after their initiation but become stable after a while, moving to a steady state. Other processes fluctuate on a scale that is often much smaller than necessary to include in the analysis of such systems. An averaging approach is then taken, resulting in steady-state analysis. The steady state is also assumed when the analysis period is so short that temporal effects are not noticeable.

Table 1. Summary of mechanisms tending to produce fluctuations in groundwater levels (Freeze and Cherry 1979)

	unconfined	confined	natural	man-made	short-lived	diurnal	seasonal	long-term	climate influence
- Groundwater recharge (infiltration to water table)	x		x			x	x		x
- Air entrapment during groundwater recharge	x		x		x				x
- Evapotranspiration and phreatophytic consumption	x		x			x			x
- Bank storage effects near streams	x		x				x		x
- Tidal effects near oceans	x	x	x			x			x
- Atmospheric pressure effects	x	x	x			x			x
- External loading of confined aquifers		x		x	x				
- Earthquakes		x	x		x				
- Groundwater pumpage	x	x		x				x	
- Deep well injection		x		x				x	
- Artificial recharge: leakage from ponds, lagoons, landfills	x			x				x	
- Agricultural irrigation and drainage	x			x			x	x	x
- Geotechnical drainage of open pit mines, slopes, tunnels, excavation sites	x			x				x	

Dimensions in the time domain range from millenia in paleohydrological simulations and risk analysis for long-term isolation of radioactive waste through year by year, to seasonal, monthly, weekly, daily, and hourly scales for field systems, to modeling of real-time systems on a basis of minutes and even seconds in some laboratory experiments.

Scales in groundwater hydrology can be viewed from two perspectives. First is the physical scale on which the hydrological processes take place (Figure 4, Table 2). These processes provide the physical setting in which human interaction can be studied, as they occur in unintentional or managed alterations in the natural system (van der Heijde 1988). The scale on which hydrological processes are analyzed often differs between the various subsystems of the hydrological cycle, dependent on the system's physical characteristics and on the study objectives. Furthermore, analyses of the principal features of the subsystems often requires a hierarchical discretization that differs between the subsystems. Among other cases, this is the case between the atmospheric and subsurface processes in watershed response to precipitation patterns, and between soils and aquifers for analysis of flow and pollutant transport. Another perspective is that of resource management, where socioeconomic and political conditions are paired with the hydrological and engineering aspects of a groundwater system.

In general, human-induced influences on groundwater systems affect local and intermediate scales, while large, regional-scale phenomena are of natural origin. Some human-induced changes are also on a regional scale, such as the amalgamated effect on water levels and return flow of groundwater withdrawal for irrigation; nonpoint pollution caused by use of fertilizers, herbicides, and pesticides in agriculture; acidification of groundwater as a result of acidic precipitation; and the changes in quality resulting from urbanization.

From a management point of view a system can be hierarchical, divided into administrative elements such as townships, counties, states, and river basins. If modeling is intended to provide optimal courses of action in the management of the water resources, an approach based on administrative elements can be successful. However, such an approach does not follow natural boundaries and elements and therefore, often, does not accurately consider the effect of physical processes and stresses occurring outside the administrative area.

In many management situations, selection of the scale of analysis is influenced by the restrictions in data availability. In part, such restrictions are imposed by the lack of techniques for obtaining higher-resolution data. For example, in groundwater modeling the recharge term of the subsurface water balance is directly related, through precipitation and evaporation, to atmospheric processes and conditions. These exchange variables between atmosphere and soil surface are obtained either through direct measurement (rainfall) or indirectly through calculation (evaporation), using various atmospheric variables. Such data were formerly available only for a limited number of sampling stations. Consequently, such stations are considered to represent a rather large area, thus limiting severely the accuracy with which the recharge can be determined. In recent years remote sensing has developed as a promising means for obtaining areal values for a number of significant parameters (e.g., soil moisture and snow cover).

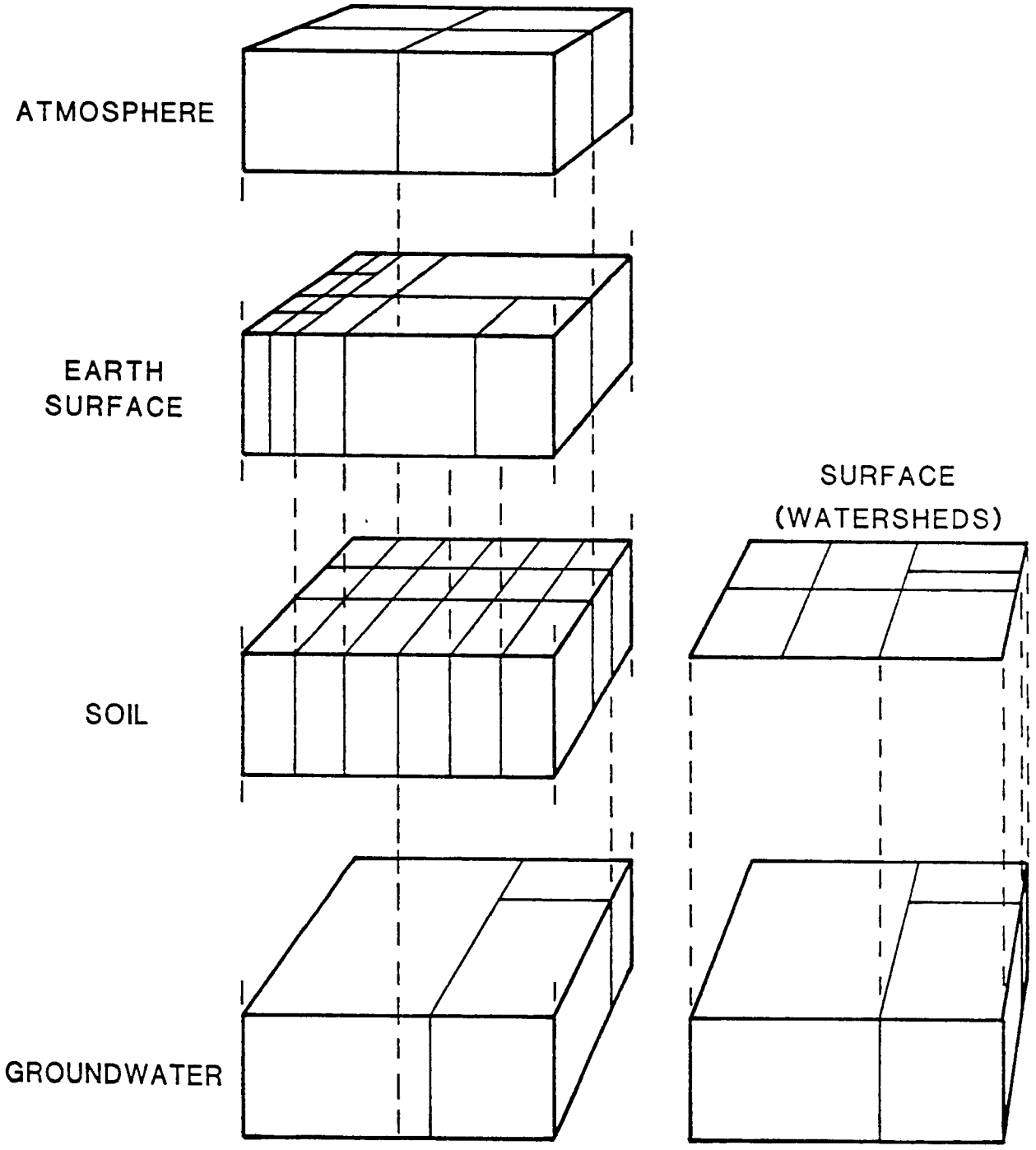


Fig. 4. Scales and relative sizes of various hydrological systems (after van der Heijde 1988).

Table 2. Scales in groundwater modeling (van der Heijde 1988).

	Site	Local	Intermediate	Regional
area	<100m	100-1000m	1000-10000m	>10,000m
examples	tracer test, pumping test	point source, pollution, small well fields	small aquifers, large point-source pollution	basins large aquifers, nonpoint pollution
geology	homogeneous	single horizontal unit; some vertical layering	a few horizontal units and significant vertical layering	heterogeneous in both horizontal and vertical directions
flow	single aquifer or part of aquifers; homogeneous, possibly anisotropic	single aquifer or part of aquifers; homogeneous, possibly anisotropic	single or multiple aquifer(s); heterogeneous in horizontal direction, anisotropic, possibly some vertical layering	multiple aquifers; heterogeneous, anisotropic, vertically layered
solute transport	homogeneous	homogeneous in horizontal direction, layered	heterogeneous, layered	heterogeneous, layered

Spatial Scales

Water supply problems are generally related to availability of sufficient water to cover water needs, and to drawdown of groundwater levels and reduction of pressures and storage as a result of the exploitation of the resource (van der Heijde 1988). Industrial and municipal water supply requires wellfields with the wells relatively closely spaced (50-200 m) in order to obtain an efficient connection with the distribution network. Their area of influence can range from less than 1 km^2 to more than 100 km^2. Private, single-household wells have a small area of influence (often less than 100 m in radius), but individual irrigation wells may have a significant influence on a system (up to a few thousand meters). In some areas the combined drawdown of a large number of private wells can cause serious aquifer depletion. This is especially true with agricultural water use. The total effect of large-scale irrigation from groundwater may lower the water levels in entire aquifer systems, e.g., the long-term depletion of the Central Valley aquifers in California, and of the Ogallala aquifer in the High Plain region. This problem occurs most often in areas with low to moderate recharge from precipitation.

Groundwater pumpage aimed at lowering water levels may assume large-scale proportions, as with dewatering for mining operations. An example is the open-pit mining of lignite in the northern part of the Rhenish lignite mining district of West Germany, where drawdowns of more than 100 m occur to keep the pit dry. The influence of this dewatering is felt more than 20 km off-site, and the affected area is still expanding as a result of continuing dewatering (Boehm 1983).

Operation of groundwater systems and conjunctive management of coupled groundwater-surface water systems have their special scale requirements, ranging from the scale of a major watershed or river basin (for policy decisions) to that of sections of the aquifer or stretches of the river (for local planning and engineering purposes).

So-called human-induced point-source groundwater contamination, as from spills, leaching from landfills or lagoons, and underground tank failures, often occurs on a much more local scale (100-1000 m). However, if nothing is done about such groundwater deterioration, the affected area can become quite extensive (1000-10,000 m).

Some basins are affected by a large group of individual point sources such as septic tanks or landfills and dumps. The aggregated effect of these is comparable with that of nonpoint pollution. In such cases, individual mitigation has no effect and regulatory action for the entire basin is required.

Related to the discussion of spatial scales in groundwater systems is the phenomenon of hydrogeologic heterogeneity or nonuniformity. Various types of heterogeneity exist: layered, discontinuous, and trending hetrogeneity (Freeze and Cherry 1979). Layered heterogeneity occurs in sedimentary deposits, while discontinous heterogeneity, also found in sedimentary deposits, is caused by faults or large-scale stratigraphic features. The last class, trending heterogeneity, exists within similar geologic formations in response to sedimentation processes. These classes of heterogeneity may be treated deterministically. Uncertainty exists, however, due to the lack of information about the

system or to the variable nature of certain properties or processes. As discussed by Dettinger and Wilson (1981), uncertainty results from the absence of enough or accurate information about the system but may be reduced through measurements. Intrinsic uncertainty (i.e., due to variability) is caused by small-scale fluctuations superimposed on deterministic, large-scale variations. The small-scale fluctuations contain smaller fluctuations, and so forth. Intrinsic uncertainty is a physical variability, and in contrast to information uncertainty, cannot be reduced by measurements. However, the accuracy of characterizing the physical variability increases by increasing the number of observations. Through the use of widespread measurements, descriptions of the intrinsic variability in a field system can help reduce information uncertainty.

Temporal Scales

For water management purposes, temporal scales are important. Incidental local situations, such as construction site dewatering and chemical spills, have mainly short-term effects for weeks or months. Seasonal effects are related to agricultural uses and the use of aquifers as thermal energy sources or storage. Mid- to long-term scales (1-20 years) apply to many wellfield operations, dewatering of mining sites, and local pollution problems. Long-term effects (20-100 years) are of special interest in regional water resource development, hazardous waste displacement, and regional nonpoint pollution. Historical periods (100 years to millions of years) are of interest for paleohydrogeological studies and for isolation of highly toxic, nondegradable chemicals and long-living radionuclides.

A typical example of temporal scales as applied in groundwater models is the study of the South Platte River in Colorado (Morel-Seytoux and Restrepo 1985). This model currently simulates about a 160 km stretch of river and hydraulically connected aquifer. The model is used for two types of analysis: (1) daily operation of the conjunctive use river-aquifer system, aimed at allocation of irrigation water according to availability and water rights, and (2) evaluation of policies and legislation. In the operational mode a daily simulation time-step is used for the surface water system and a weekly simulation is used for the groundwater away from the river. To account for the more rapid responses of the groundwater near the river, a correction is made to the results of the weekly simulations for the parts of the aquifer along the river. For the use of the model in the development of policies and in evaluating new legislation, as in the formulation of new water distribution rules, the scale is much larger because long-term effects are of interest. In the South Platte River study, a weekly timestep is used for surface water, a monthly timestep for groundwater.

In planning remedial action, temporal scales are directly dependent on the extent of the polluted area, the geology, the important hydrological and biochemical processes, and the remedial action itself. For example, remedial actions designed for control of erosion and runoff, such as grading and surface water diversion, could require transient simulation with short timesteps for the rainfall and runoff processes that fluctuate rapidly (daily scale). In the saturated zone the flow is more regular and changes occur within a time frame of months or even years. Dynamically linked submodels, each with its own time scale, are then required for efficient simulation. To evaluate the threat of pollution to humans and the environment, or to analyze the effects

of remedial action, simulation periods of 20-100 yrs are common. Much longer-term effects may have to be included, as in the case of long-living radionuclides and chemically inert toxic organics.

An example of temporal scale is radioactive waste storage in unsaturated systems, where effects must be evaluated for time periods up to 10,000 yrs (EPA 1982). Because of the strongly nonlinear character of the flow and transport equations for the unsaturated zone, the timesteps cannot be too large (Reisenauer et al. 1982, Tripathi and Yeh 1985). Tripathi and Yeh (1985) used variable time steps up to 20,000 yrs to simulate an unsaturated system for such an extended time.

3. MODEL DEVELOPMENT

In groundwater modeling a distinction is often made between two major categories of activities: model development and model use in management. Model development consists of researching the quantitative description of the groundwater system, a software development component, and model testing. Model development is closely related to the scientific process of increasing knowledge: observing nature, posing hypotheses for the observed information, verifying the proposed relationships, and thus establishing a credible theoretical framework and improving our understanding of nature. Model development is often driven by the short-term and less frequently by the long-term needs of natural resources management. The resulting, often-generic computer codes are used in model application as part of a larger set of activities which included data collection and interpretation, technical design, economical evaluation, and so forth. The present chapter discusses the model development processes (Figure 5) and related issues, while Chapter 4 discusses the model application process.

THE MODEL DEVELOPMENT PROCESS

The development and use of models encompasses a broad spectrum of technical expertise. At one end is management; at the other end is scientific research. Between are two principal categories: model builders engaged in the development of models, and technical experts concerned with their operational use (Bachmat et al. 1978). The four categories are not rigidly separated. However, considering the categories as distinct helps elucidate the general framework of model development and use and of modeling-related problems.

The roots of model building lie in research. The fundamental understanding of a groundwater system is the product of research synthesized by theory. The object of such research is a prototype natural system containing selected elements of the real world multi-element groundwater resources systems. The selection is driven by management needs and the researcher's interest, and is influenced by the initial, often cursory conceptualization based on sampling of the real-world system (Figure 6). The conceptual model of the groundwater system thus derived forms the basis for determining the causal relationships among various components of the system and its environment. These relationships are defined in mathematical terms, resulting in a mathematical model. If the solution of the mathematical equations is complex, as with some closed-form analytical solutions (see Chapter 5), or when many repetitious calculations are necessary, as with numerical solutions, the use of computers is essential. This requires the coding of the solution to the mathematical problem in a programming language, resulting in a computer code. The conceptual formulations, mathematical descriptions, and the computer coding together constitute the prototype model (Figure 6).

In model development, the next step is code testing. This important phase is aimed at removing programming errors, testing embedded algorithms, and evaluating the operational characteristics (e.g., input/output facilities, user friendliness, efficiency; see code selection section of Chapter 4) of the code through its execution on carefully selected example datasets (Adrion

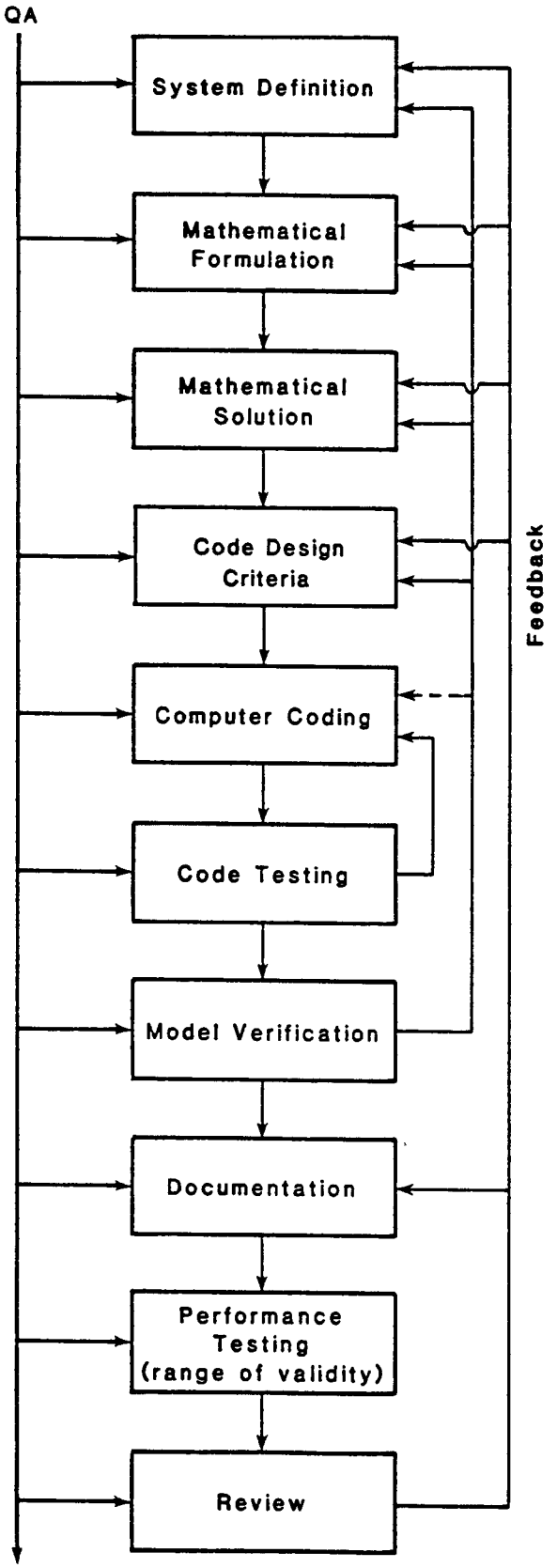


Fig. 5. Model development process and feedback.

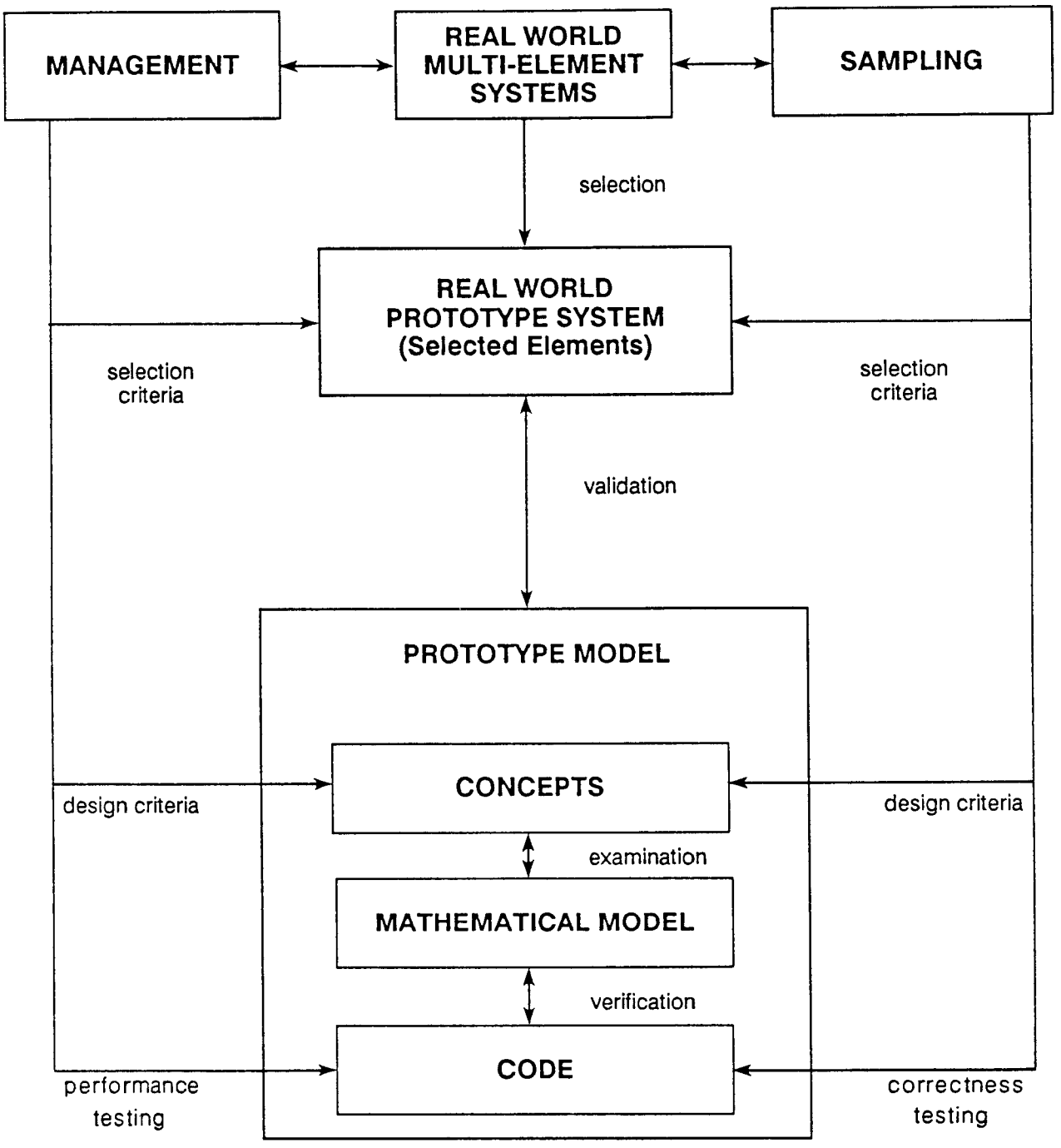


Fig. 6. Model development concepts.

et al. 1986). This stage is often called code verification and is closely related to the scientific process of model verification in which the evaluation of the operational characteristics of the code is extended to its mathematical formulation and solution (assuming a good understanding of the system, its components, and the interrelationships between the individual system components). Many research publications report on work done up to this point in the model development process. Finally, data independently derived from field sites are used, if available, to establish the code's performance and validity for particular types of application by assessing the closeness of the computed results to the system the model is supposed to simulate. In this case, the selected code is an integral part of the model (concepts, mathematical descriptions, data) tested. However, for most types of groundwater models and applications, no such comprehensive, high-quality test datasets are currently available to confirm the validity of the model in simulating a particular system of interest (van der Heijde 1987a). A detailed discussion of the validation process is presented at the end of this chapter.

As a set of simplifying assumptions, equations, and boundary conditions cast in the form of a computer code, the model may hardly be operational. Accurate instructions are needed for the preparation of datasets that will form the input for the code. Therefore, the next stage in the development of an operational model—the preparation of documentation—is an important step in the establishment of the code's utility. Documentation should consist of sections on theory, code structure, operational environment, testing and use. The instructions contained in the documentation should cover such topics as hydrogeologic schematization, selection of boundary conditions, gridding and parameter selection (van der Heijde 1987a). With proper documentation, the code can be externally evaluated, a quality control procedure that includes independent review of theory, code, and documentation, audit of the model development process, and additional performance testing (establishing the range of parameters, stresses, and scales for which the model can be used successfully).

When all these steps have been taken, the code is operational and ready to apply to management problems. In the course of its use, the code gains confidence by proving its reliability and applicability. This can be further improved by provisions for continuing support and maintenance. It should be noted that when changes are made in the code or when model characteristics or model features are modified, the review and testing process must be repeated rigorously.

Not all simulation codes resulting from research into the physical and chemical processes of groundwater systems reach this final stage. This is partly due to the objectives of the research and development and in part to the way the project has been launched, or initialized. Basically, three courses of action are possible: (1) codes can be developed primarily as research tools (such codes frequently are considered experimental and are not prepared or released for external use); (2) codes can be developed to provide practical, descriptive, and predictive management tools for solving field problems (this type of code is often developed at the special request of planning, management, or enforcement agencies); and (3) codes can be developed by consultants as an investment for future consultancy. Codes from the last two groups are often based on codes of the first category, generally come with some form of documentation, and have undergone at least limited testing.

MODEL VALIDATION

Successful water management requires that decisions be based on the use of technically and scientifically sound data collection, information processing, and interpretation methods and that these methods are properly integrated. As computer codes are essential building blocks of modeling-based management, it is crucial that before related computer codes are used as planning and decision-making tools, their credentials must be established, independently of their developers, through systematic testing and evaluation of the codes' characteristics. As in the case of the nuclear industry (Bryant and Wilburn 1987), software applications in groundwater protection have become too prominent for the codes to be developed and maintained in the informal atmosphere that was common in early groundwater modeling software development. Therefore, determining the validity of a code for modeling well-defined groundwater systems as part of an analysis of the influence of anthropogenic stresses on such systems is a crucial step in the development of software to be used in environmental decisionmaking. It is important at this stage of the discussion to make the distinction between code testing and model testing. Code testing is limited to establishing the correctness of the code with respect to the criteria and requirements for which it is designed. Model testing is more inclusive, as it extends to establishing the model's closeness to the real-world systems it is designed to simulate (Figure 6).

Definitions and Methods

Determining the correctness of a model is basically part of the scientific discovery process and as such is a rather subjective process. When will a model, or for that matter a theory, be accepted by the scientific community? Such acceptance is a gradual process. On the other hand, code validation can be more objective and precise. The proof of a code's correctness in representing a model of the real system can be obtained by using logic to infer that an assertion assumed true at program entry is also true at program exit (Adrion et al. 1986). There are various ways to obtain such a proof, e.g., code verification.

Much confusion has resulted from equating model validation with code validation and model verification with code verification. The term "validation" is defined according to the discipline in which it is used. In terms of software engineering such as adopted by the National Bureau of Standards, code validation is defined as "the determination of the correctness of the final software product with respect to user needs and requirements" (Adrion et al. 1986). Code validation is sometimes called "functional testing" of software. In discussing standard practice for evaluating environmental fate models of chemicals, ASTM (1984) defines model validation as "the comparison of model results with numerical data independently derived from experiments or observations of the environment."

A term closely related to validation is verification. In software engineering, verification is the process of demonstrating consistency, completeness, and correctness of the software (Adrion et al. 1986). ASTM (1984) defines verification as the examination of the numerical technique in the computer code to ascertain that it truly represents the conceptual model and that there are no inherent problems with obtaining a solution.

Combining code testing with code review provides a more comprehensive evaluation. In this type of assessment of code quality its actual characteristics, established through examination and measurement, are compared with required characteristics. To be conclusive in model review and testing the code design criteria and the test criteria must be defined explicitly. Software engineering distinguishes various methods of examination (Schmidt et al. 1988): (1) static analysis to establish the correctness of the program's syntax; (2) dynamic analysis to evaluate for correct results, correct operations, efficiency in time, and efficiency in storage capacity; and (3) verification and symbolic execution to establish the correctness of algorithms. Quantitative assessment of the quality of the software is normally done by measuring the code's performance.

The following discussions follow the ASTM definitions as closely as possible.

Thus, the objective of groundwater model validation is to determine how well a model's theoretical foundation and computer implementation describe actual system behavior in terms of the "degree of correlation" between model calculations and actual measured data for the cause-and-effect responses of prototype groundwater systems. Various methods exist to quantify or describe qualitatively this degree of correlation. It should be noted that the actual measured data of both model input and system response are samples of the real system and inherently incorporate errors. Thus, model validity established in this manner is always subjective (measured validity; Figure 7).

To determine the validity of a groundwater model we need to answer such questions as (Figure 6):

- Is the conceptual model valid for the prototype system (as defined in the beginning of this chapter) it represents? Related to this question is the purpose for which the model will be used; different levels of simplification or detail might be sufficient or required to fulfill the designer's or user's objectives.

- Does the mathematical model truly represent the conceptual model, the processes involved, and the stresses present for the various design conditions?

- Does the code currently represent the mathematical framework?

It should be noted that in applying a model, the validity of its predictions needs to be established, requiring additional criteria and assessment methods (see Chapter 4: Model Application).

Four testing approaches are available to determine the validity of a model in simulating a particular groundwater system: calibration, extended field comparison (often called field validation), code intercomparison, and post-audits.

The validity of groundwater models is preferably assessed on the basis of the simulation of a well-defined field experiment or highly detailed field exploration study, sometimes backed up with well-conditioned laboratory experiments. Comparing the predicted with the measured responses may take

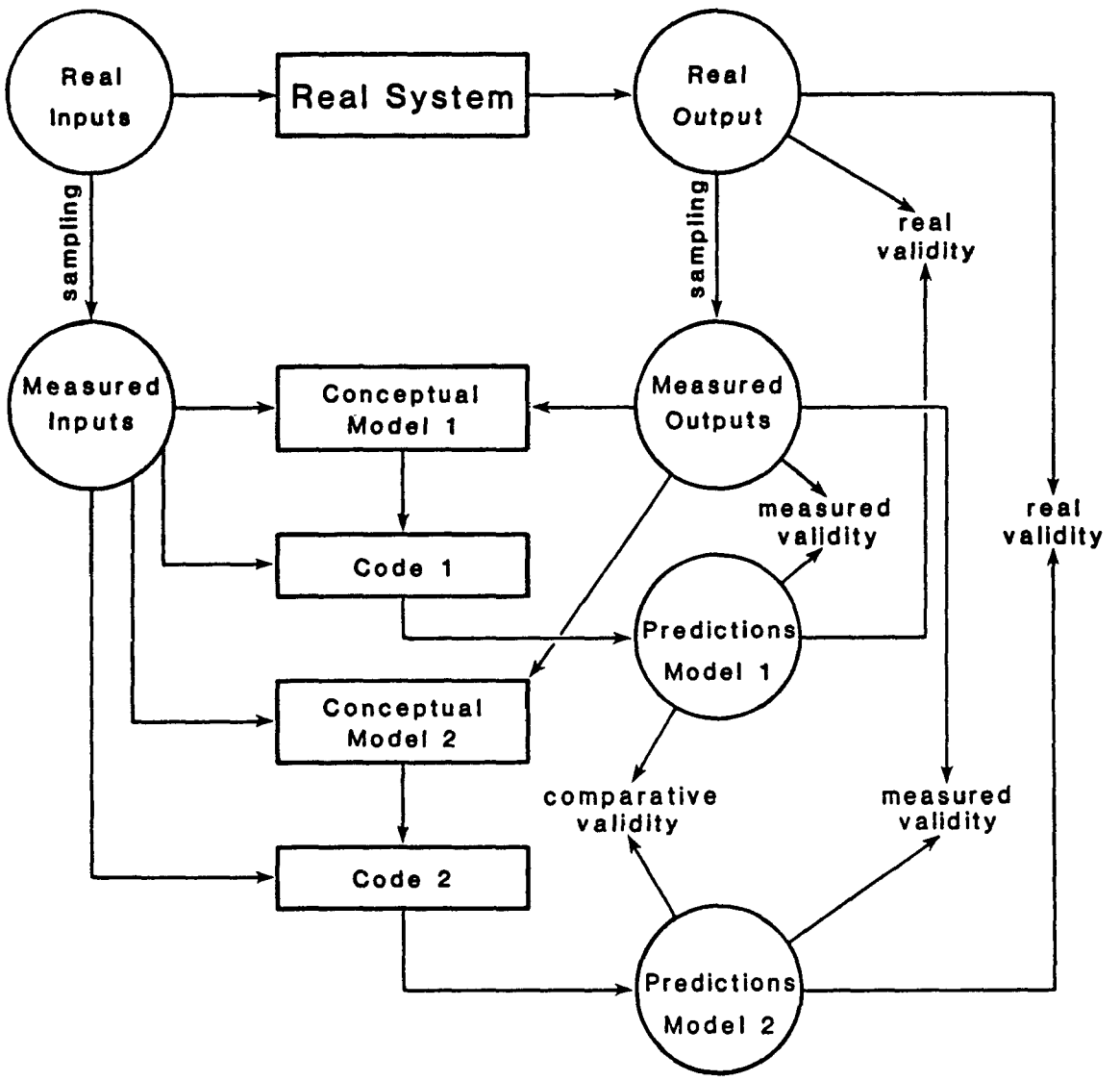


Fig. 7. Assessing model validity.

either of two forms. One form, calibration, is sometimes considered the weaker form of validation insofar as it tests the ability of the code (and the model) to fit the field data, with adjustments of the physical parameters (Ward et al. 1984). Some researchers prefer to classify calibration as a form of verification rather than a form of validation, as calibration does not provide for testing independently of the model's coding (van der Heijde 1987a). The results of the calibration runs might be influenced by model or code errors if still present.

A more rigorous form of validation is testing the model's ability to match the experimental data, using modeling-independent estimates of the parameters. In principle, this is the most extensive approach to validation. However, unavailability and inaccuracy of field data often prevent applying such a rigid validation approach to actual field systems. Typically, a part of the field data is designated as calibration data, and a calibrated site-model is obtained through reasonable adjustment of parameter values. Another part of the field data is designated as validation data; the calibrated site model is used in a predictive mode to calculate system responses for comparison. The quality of such a test is therefore determined by the extent to which the site model is "stressed beyond" the calibration data on which it is based, i.e., represents the same system conditions and stresses for which it has been calibrated (Ward et al. 1984). The primary value of calibration as a model testing tool is that failure in calibrating a model to a field site might indicate for incorrect model formulation or coding errors. In this report, this type of partial validation is called field testing.

As mentioned before, only a few datasets are currently available for testing most kinds of groundwater models. These datasets are limited with respect to the variety of conditions and stresses that occur in the sampled system. System conditions or stresses needed for a full range of validity determinations are technically or financially often not feasible to realize or are restricted by regulation or other legal constraints. Therefore, testing of models is generally limited to extended verification using existing analytical solutions, to code intercomparison, and to post-audits of model applications.

An additional complexity is that often the data used for field validation are not collected directly from the field by the model development team but are processed in an earlier study. Therefore, they are subject to inaccuracies, loss of information, interpretive bias, loss of precision, and transmission and processing errors, resulting in a general degradation of the data to be used in the validation process. For these reasons, "absolute" validity of a model does not exist and only a "limited," "partial" or "relative" validity can be established.

Another weak form of validation is found in the performance of post-audits, studies performed after the system is actually stressed according to simulated scenarios where the observed results are compared with the original predictions. To use post-audits successfully in determining model validity, conceptualization, assumptions, and system parameters and stresses should be updated and the model rerun to facilitate comparison of predictions with recent, observed system responses. Although post-audits are used primarily to determine the rate of success of a model application, if a post-audit concludes that the initial predictions were reasonable and that inaccuracies in

the initial predictions were caused primarily by insufficient or inaccurate data, such a study contributes to the acceptability of the model itself.

Another, weaker form of validation is found in code intercomparison. This type of testing is often aimed at establishing relative performance characteristics of various codes, using an existing dataset. However, if such datasets are not available, a newly developed model might be compared with established models designed to solve the same type of problems as the new model, using hypothetical problems and generic datasets. If the simulation results from the new code do not deviate significantly from those obtained with the existing code, a "relative" or "comparative" validity is established (Figure 7). However, if significant differences occur, in-depth analysis of the results of simulation runs performed with both codes is called for. If code intercomparison was used to evaluate a new code, all the models involved should again be validated as soon as adequate datasets become available.

Whether a model is valid for a particular application can be assessed by a careful selection process that includes applying predetermined performance criteria, sometimes called validation or acceptance criteria (see Section 4). If various uses in planning and decision making are foreseen, different performance criteria might be defined. The user should then carefully check the validity of the model for the intended use. In this context, acceptance is sometimes cast in terms of software or model certification. Software engineering usually considers certification as acceptance of software by an authorized agent after the software has been validated by the agent or after its validity has been demonstrated to the agent (Adrion et al. 1986). This concept has been forwarded by some agencies with respect to environmental models. However, it is far from being accepted by the scientific community. It should be noted that acceptance by an agency of software developed under contract and subsequent public release (e.g., as might be required under the Freedom of Information Act) does not constitute such certification unless all criteria, if published, have been satisfied and recorded.

Complete model validation requires testing over the full range of conditions for which the code is designed. Model development is an evolutionary process responding to new research results, developments in technology, and changes in user requirements. Model validation needs to follow this dynamic process and should be applied each time the model (or code) is modified.

Validation Criteria

In describing the degree of validity of a model as discussed above, three levels of validity can be distinguished (ASTM 1984):

(1) Statistical Validity: using statistical measures to check agreement between two different distributions, the calculated one and the measured one; validity is established by using an appropriate performance or validity criterion.

(2) Deviative Validity: if not enough data are available for statistical validation, a deviation coefficient DC can be established, e.g.,

$$DC = [(x-y)/x]100\%$$

where x = predicted value and y = measured value. The deviation coefficient might be expressed as a summation of relative deviations. If ED is a deviative validity criterion supplied by subjective judgment, a model can considered to be valid if DC < ED.

(3) Qualitative Validity: using a qualitative scale for validity levels representing subjective judgment: e.g., excellent, good, fair, poor, unacceptable. Qualitative validity is often established through visual inspection of graphic representations of calculated and measured data (Cleveland and McGill 1985).

The aforementioned tests apply to single variables and determine local-or-single variable validity; if more than one variable is present in the model, the model should also be checked for global validity and for validity consistency (ASTM 1984). For a model with several variables to be globally valid, all the calculated outputs should pass validity tests (e.g., heads, fluxes and water balances in flow models). Validity consistency refers to the variation of validity among calculations having different input or comparison datasets. A model might be judged valid under one dataset but not under another, even within the range of conditions for which the model has been designed or is supposedly applicable. Validity consistency can be evaluated periodically when models have seen repeated use.

Validation Scenarios

Often, various approaches to field validation of a model are viable. Therefore, the validation process should start with defining validation scenarios. Planning and conducting field validation should include the following steps (Hern et al. 1985):

(1) Define data needs for validation and select an available dataset or arrange for a site to study;

(2) Assess the data quality in terms of accuracy (measurement errors), precision, and completeness;

(3) Define model performance or acceptance criteria;

(4) Develop strategy for sensitivity analysis;

(5) Perform validation runs and compare model performance with established acceptance criteria;

(6) Document the validation exercise in detail.

Validation Databases

Further development of databases for field validation of models, especially solute transport models, is necessary. This is also the case for many other types of groundwater models. These research databases should represent a wide variety of hydrogeological situations and should reflect the various types of flow, transport, and deformation mechanisms present in the field. The databases should also contain extensive information on hydrogeological, soil, geochemical, and climatological characteristics. With the development

of such databases and the adoption of consistent model-testing and validation procedures, comparison of model performance and their reliability in groundwater resource management can be improved considerably.

4. MODEL APPLICATION

THE MODEL APPLICATION PROCESS

The effective application of computer simulation models to field problems is a qualitative procedure, a combination of science and art. A successful model application requires knowledge of scientific principles, mathematical methods, and site characterization, paired with expert insight into the modeling process. These elements often are provided in a multidisciplinary team framework. Modeling imposes discipline by forcing all concerned to be explicit on goals, criteria, constraints, relevant processes, and parameter values (European Institute for Water, Modeling for Water Management, Workshop Statements, May 21-22, 1987, Como, Italy).

The preparation of an operational model of a groundwater system can be divided into three distinct stages: initialization and preparation, calibration, and problem solving or scenario analysis (sometimes called prediction stage; Figure 8). Each stage consists of various steps; often, results from a certain step are used as feedback in previous steps, resulting in a rather iterative procedure.

The modeling process is initiated with the formulation of the modeling objectives and modeling scenarios derived from an analysis of the management problem under study. Within this context, compilation, inspection, and interpretation of available data result in a first conceptualization of the system under study. Often, the technical expert is charged with the task of making sense of an ill-posed problem with a large amount of mostly irrelevant data. It is his/her task to rationalize the ill-posed problem into an unambiguous question that, to be answered, utilizes a subset of the data available together with data specifically collected to solve the problem. (Cross and Moscardini 1985).

Conceptualization of a groundwater system consists of three elements: (1) identification of the state of the system; (2) determination of the system's active and passive controls; and (3) analysis of the level of uncertainty in the system (Kisiel and Duckstein 1976). To identify the state of the system, its hydraulic, chemical, thermal, and hydrogeologic characteristics are defined, and conservation of mass, energy, and momentum are quantified. The active input refers to such system controls and constraints as pumpage schedules, artificial recharge, development of new well fields, waste injection rates, and the construction of impermeable barriers, and clay caps and liners. If the studied system includes economic or decision-making policy aspects, active input may also include interest rates, pumping and waste generation or waste disposal taxes, and policies for conjunctive use. Passive or uncontrollable inputs include elements of the hydrologic cycle external to the system under study, such as natural recharge and evapotranspiration, subsidence, and natural water quality. Certain contamination sources such as leaching landfills, spills, and the leaching of agricultural chemicals present in soil might also be considered as passive controls. Other passive controls, such as water demand resulting from population growth, may be external management factors.

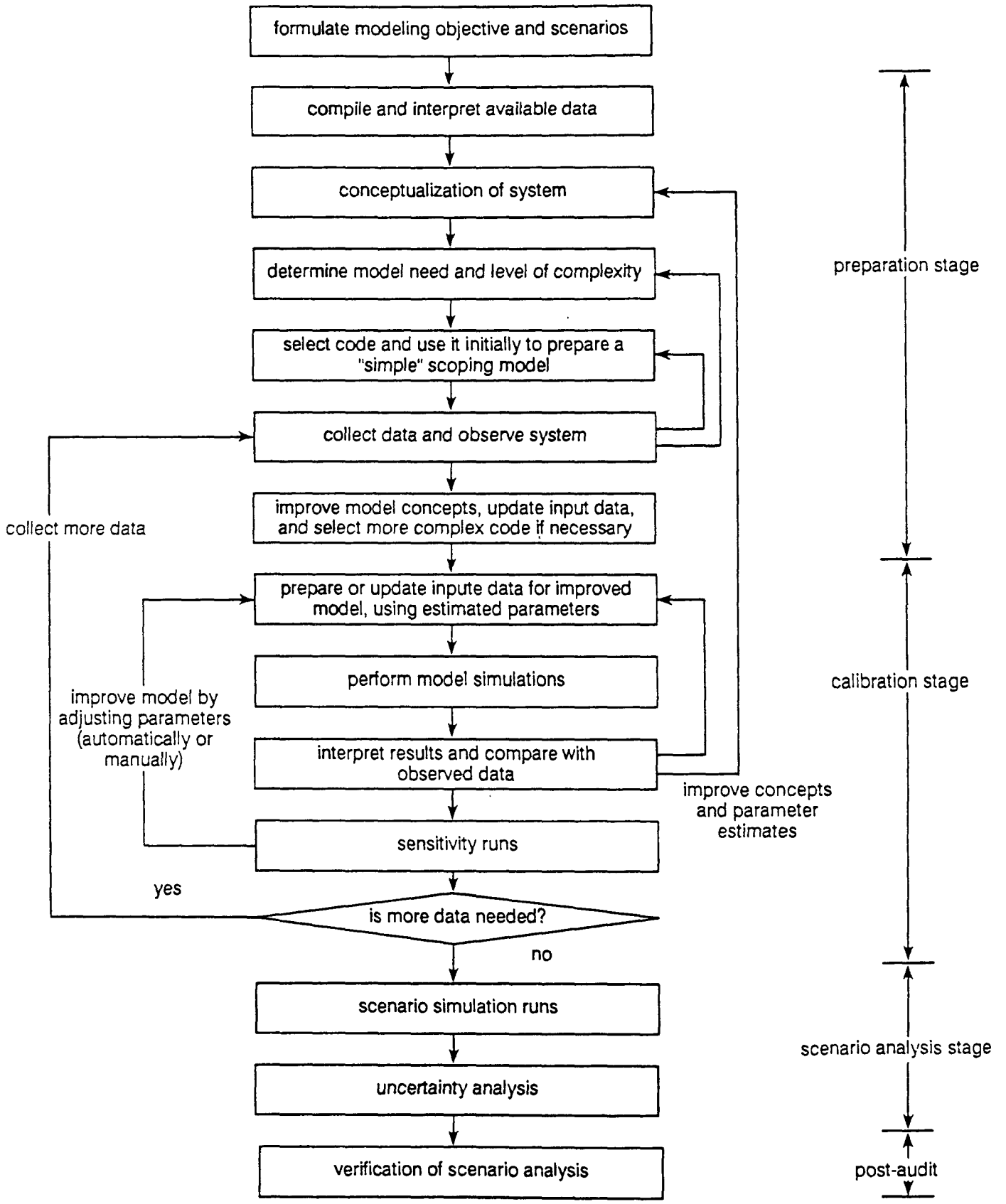


Fig. 8. Model application process.

Many modeling studies found to be inadequate were hampered by deficiencies in the analysis of the problem to be modeled or in the conceptualization of the groundwater system (van der Heijde and Park 1986).

Based on the objectives of the study and the characteristics of the system, the need for and complexity level of the simulation model must be determined. Selection of a computer code takes place; if the code is new to the technical staff, they need some time to become familiar with its operational characteristics.

The second stage of model application, calibration, starts with the design or improvement of the model grid and the preparation of an input file by assigning nodal or elemental values and other data pertinent to the execution of the selected computer code. The actual computer simulation then takes place, followed by the interpretation of the computed results and comparison with observed data. The results of this first series of simulations are used to further improve the concepts of the system and the values of the parameters. Sensitivity runs are performed to assist in the calibration procedure. More data may be needed during the calibration process.

In some cases the code is used initially to design a data collection program. The newly collected data are then used both to improve the conceptualization of the system and to prepare for the predictive simulations.

After the calibration stage has been concluded satisfactorily, it is followed by the scenario analysis stage, in which the computer code is used to obtain answers to such management problems as the impacts of proposed policies, engineering designs, and system alterations. In fact, in this stage current understanding of the system is extrapolated to evaluate its response to new or altered stresses. The use of uncertainty analysis in this stage of the modeling process provides insight into the reliability of the computed predictions.

In the final stage of a model application project, the computed results are checked with respect to feasibility and completeness and analyzed in the context of the management problem being addressed. When the technical expert has finished the analysis, the key answers obtained in the modeling process are presented to management. In the modeling process, interaction between technical experts and management is often an iterative process, with management asking new questions based on the results of previous modeling-based analysis.

Whenever an opportunity exists to obtain further field information regarding the system being modeled, refinements and improvements in the model should be made and previous analysis modified. Sometimes, such an opportunity is offered in the form of post-audits. Post-audits are reviews performed some time after the model-based predictions were made and often provide an opportunity for in-depth analysis regarding the inaccuracies in those predictions. However, not many of such post-audits actually take place, depriving modelers and managers from important feedback and educational experience.

Often, a major impediment to the efficient use of models in groundwater management is the lack of data. Data insufficiencies might result from inadequate resolution in spatial data collection (e.g., spatial heterogeneities

relevant on smaller scale than sampled), or in temporal sampling of time-dependent variables (e.g., measured too infrequently), and from measurement errors (Konikow and Patten 1985).

Many types of problems can occur in the application of models. Some of these are technical, method-dependent problems such as numerical dispersion and oscillations in transport models. Conceptual problems, often significant, can be related to the mechanisms (e.g., dispersion, adsorption, multiphase or multifluid flow), the heterogeneity of the medium, or the simplifying assumptions adopted (e.g., vertical averaging). Finally, problems external to the model execution can occur, such as those caused by the absence of good data, model availability, available computer facilities, skilled professionals, and competent technicians.

CODE SELECTION

In the model application process, code selection is critical in ensuring an optimal trade-off between effort and result. The result is generally expressed as the expected effectiveness of the modeling effort in terms of forecast accuracy. The effort is ultimately represented by the costs. Such costs should not be considered independently from those of field data acquisition. For a proper assessment of modeling cost, such measures as choice between the development of a new code or the acquisition of an existing code, the implementation, maintenance, and updating of the code, and the development and maintenance of databases, need to be considered.

The Code Selection Process

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

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

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

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

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

The major model-oriented criteria in model selection are: (1) that the model is suitable for the intended use; (2) that the model is reliable, and (3) that the model can be applied efficiently (van der Heijde and Beljin 1988). The reliability of a model is defined by the level of quality assurance applied during its development, its verification and field validation, and its acceptance by users. A model's efficiency is determined by the availability of its code and documentation, and its usability, portability, modifiability, and economy with respect to human and computer resources required.

As model credibility is a major problem in model use, special attention should be given in the selection process to ensure the use of qualified models that have undergone adequate review and testing. However, a standardized review and testing procedure has not yet been widely adopted, although various organizations have established their own procedures (van der Heijde 1987a, Beljin and van der Heijde 1987). In addition, discussions have started within Subcommittee D-18.21 for Groundwater Monitoring of the American Society for Testing and Materials (ASTM) as part of their task on design and analysis of hydrogeologic data systems (J.D. Ritchey, pers. comm. 1987).

Finally, acceptance of a model for decision-support use should be based on technical and scientific soundness, user friendliness, and legal and administrative considerations.

In selecting a code, its applicability to the management problem studied and its efficiency in solving these problems are important criteria. In evaluating a code's applicability to a problem, a good description of its operating characteristics should be accessible. For a large number of groundwater modeling codes, such information is obtainable from the International Ground Water Modeling Center (IGWMC), which operates a clearinghouse service for information and software pertinent to groundwater modeling (van der Heijde 1987b).

Although adequate models are available for analysis of most flow-related problems, this is less the case for modeling contaminant transport and other complex processes in the subsurface. For example, computer codes are available for situations that do not require analysis of complex transport mechanisms or chemistry. The use of such programs for groundwater quality assessment is generally restricted to conceptual analysis of pollution problems, to feasibility studies in design and remedial action strategies, and to data acquisition guidance. It should be noted that, considering the uncertainties

associated with the parameters of groundwater systems, much progress has been made in determining the probabilities of the arrival of a pollution front rather than the calculation of concentrations (Bear 1988). Chapter 5 gives a detailed discussion of the various models currently available for groundwater evaluations.

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

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

Further information on groundwater model selection is presented in (Rao et al. 1982, Kincaid et al. 1984, Boutwell et al. 1985, Simmons and Cole 1985).

Code Selection Criteria

Acceptance of a model should be based on technical and scientific soundness, its efficiency, and legal and administrative considerations. A model's efficiency is determined by the availability of its code and documentation, access to user support, and by its usability, portability, modifiability, reliability, and economy. A brief discussion of some of these criteria is given below and follows a more extended treatment in van der Heijde and Beljin (1988). This latter publication includes also a proposed rating system for each of these criteria.

Availability--

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

Models developed by consultants and private industry are often proprietary. This may also be true of software developed by some universities and private research institutions. Proprietary codes are in general protected by copyright law. Although the source codes of some models have appeared in pub-

lications such as textbooks, and are available on tape or diskette from the publisher, their use and distribution might be restricted by the publication's copyright.

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

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

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

User Support--

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

User-related errors can be reduced by becoming more familiar with the model. Here the user benefits from good documentation. If, after careful selection of the model, problems in implementation or execution of the model occur and the documentation does not provide a solution, the user needs help from someone who knows the code. Such assistance, called model support, cannot replace the need for proper training in model use; requests for support by model developers may assume such extensive proportions that model support becomes a consulting service or an on-the-job training activity. This potentiality is generally recognized by model developers, but not always by model users.

Usability--

Various problems can be encountered when a simulation code is implemented on the user's computer system. Such difficulties may arise from hardware incompatibilities or coding of user errors in code installation, data input, or program execution. Programs that facilitate rapid understanding and knowledge of their operational characteristics and which are easy to use are called user-friendly and are defined by their usability (van der Heijde and Beljin 1988). In such programs, emphasis is generally placed on extensive, well-edited documentation, easy input preparation and execution, and on well-structured, informative output. Adequate code support and maintenance also enhance the code's usability.

Portability--

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

Modifiability--

In the course of a computer program's useful life, the user's experiences and changing management requirements often lead to changes in functional specifications for the software. In addition, scientific developments, changing computing environments, and the persistence of errors make it necessary to modify the program. If software is to be used over a period of time, it must be designed so that it can be continually modified to keep pace with such events. A code that is difficult to modify is called fragile and lacks maintainability. Such difficulties may arise from global, program-wide implications of local changes (van Tassel 1978).

Reliability--

A major issue in model use is credibility. A model's credibility is based on its proven reliability and the extent of its use. Model users and managers often have the greatest confidence in those models most frequently applied. This notion is reinforced if successful applications are peer-reviewed and published. As reliability of a program is related to the localized or terminal failures that can occur because of software errors (Yourdon and Constantine 1979), it is assumed that most such errors originally present in a widely used program have been detected and corrected. Yet no program is without programming errors, even after a long history of use and updating. Some errors will never be detected and do not or only slightly influence the program's utility. Other errors show up only under exceptional circumstances. Decisions based on the outcome of simulations will be viable only if the models have undergone adequate review and testing. However, relying too much on comprehensive field validation (if present), extensive field testing or frequency of model application may exclude certain well-designed and documented models, even those most efficient for solving the problem at hand.

Extent of Model Use--

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

MULTIPLE SCALES IN MODELING GROUNDWATER SYSTEMS

The scales used in groundwater modeling are determined by the characteristics of the groundwater system, by the availability of data, by the nature

of the system's management, and by requirements posed by the chosen mathematical technique. These influences often include both natural and human-induced influences, such as the effects of climate, pumping, deep-well injection, and agricultural irrigation and drainage.

An important aspect of the scaling problem relates to the difference between the scale on which processes are mathematically described, and the subsequent aggregation into larger-scale formulations amenable to field analytical procedures. Small-scale descriptions are aggregated into large-scale models by applying averaging procedures. Such averaging, when applied to a statistical description of microscopic processes, is commonly used to obtain continuous hydrodynamic field equations on the macroscopic scale (e.g., Bear 1972, 1979). Although the resulting model requires less supporting field data than is required for a problem of the same physical extent, a certain amount of information regarding the real physical systems is lost. A typical example is the apparent scale dependency of field dispersion. Recent studies have related this phenomenon to the areal and vertical variability of other aquifer characteristics such as hydraulic conductivity (Gelhar and Axness 1983, Molz et al. 1983, Sudicky et al. 1985). Also, in going to larger spatial and temporal scales, variations in system characteristics that could be ignored on the smaller scale may become important. Examples are the increasing importance of heterogeneities and anisotropy as related to the geology of the system for larger spatial scales, and the effects of long-term recharge variations on the water balance of a system for long time periods. A major problem in this averaging process lies in evaluating the effects of assumptions made on the microscopic scale and the effects on the level of uncertainty in the modeling of a groundwater system. If such assumptions have to be incorporated in the macroscopic description, their formulation may be problematic. Another problem that may arise as a result of an averaging approach is that of defining the physical meaning of the resulting state variables and system parameters. Thusfar, no systematic evaluation of the consequences of this aggregation process in groundwater has been published, although an extensive database is available to carry out such a study.

The essential scaling problem is how to distinguish between the variables that can be considered as constants or as being uniform across discrete intervals of pertinent dimension (space, time), and the variables that cannot be so considered (Beck 1985). Problem decomposition in space or time is often applied to obtain optimal resolution in relation to computational efficiency. An example of such spatial and temporal decomposition is found in the modeling of infiltration into the soil and subsequent percolation toward the saturated zone. A distinction has been made between spatial discretization and connectiveness for local (Figure 9a) and for regional (Figure 9b) scales (van der Heijde 1988). Runoff from precipitation is split into a surface component (lumped horizontal segment) and infiltration (one-, two-, or three-dimensional, vertical). The infiltrated water percolates to the groundwater where a two-dimensional horizontal or three-dimensional model is used. For each of the submodels a different timestep is used, from hourly for the surface runoff and daily for the percolation, to weekly or monthly for the flow in the saturated zone.

In groundwater models, a significant distinction exists between local and regional discretization of the surface zone. This distinction reflects the difference in physiographic character between the subsurface and the surface,

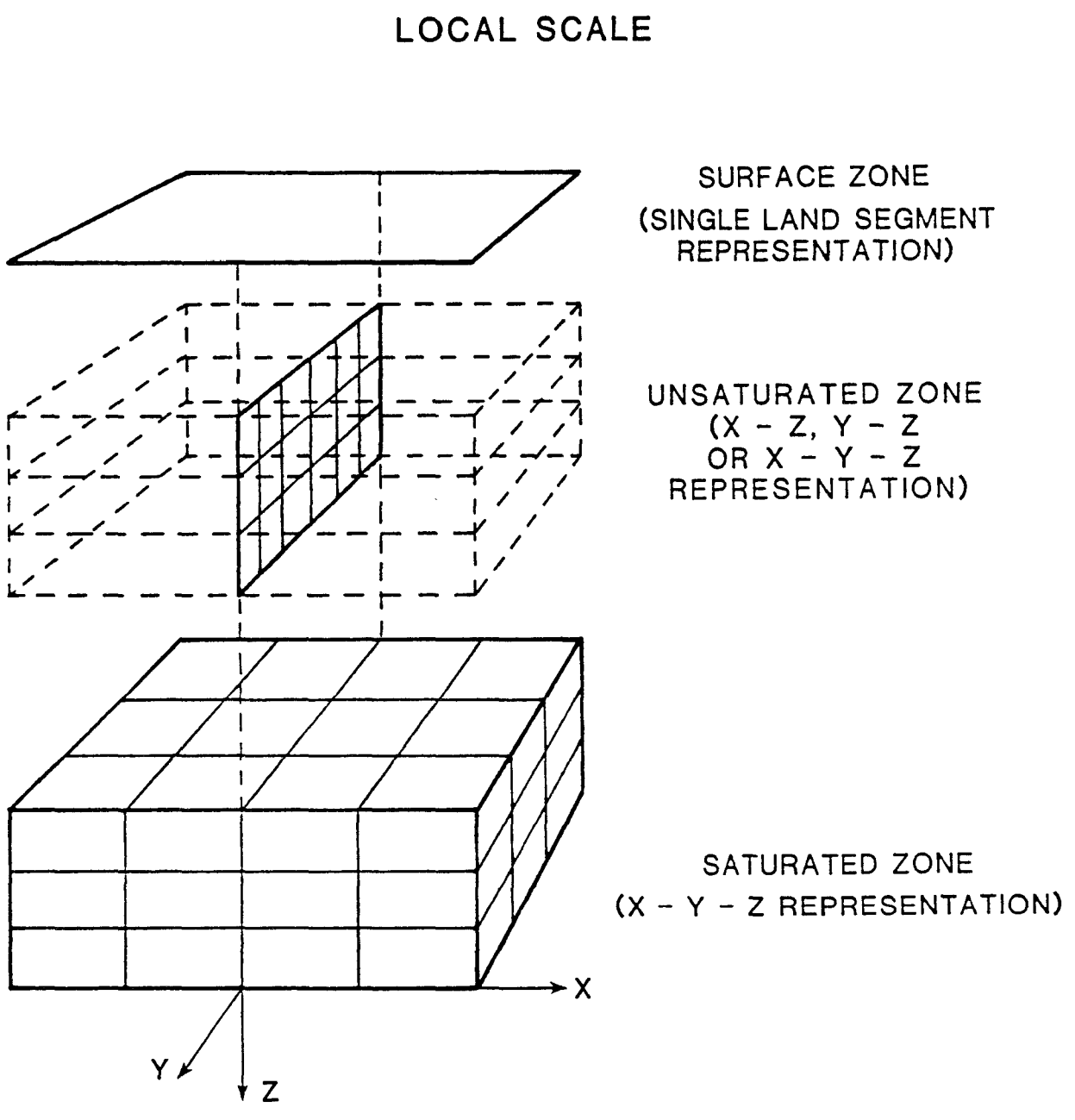


Fig. 9a. Typical dimensionalities used to represent surface, usaturated, and saturated zones in local-scale groundwater models (after van der Heijde 1988).

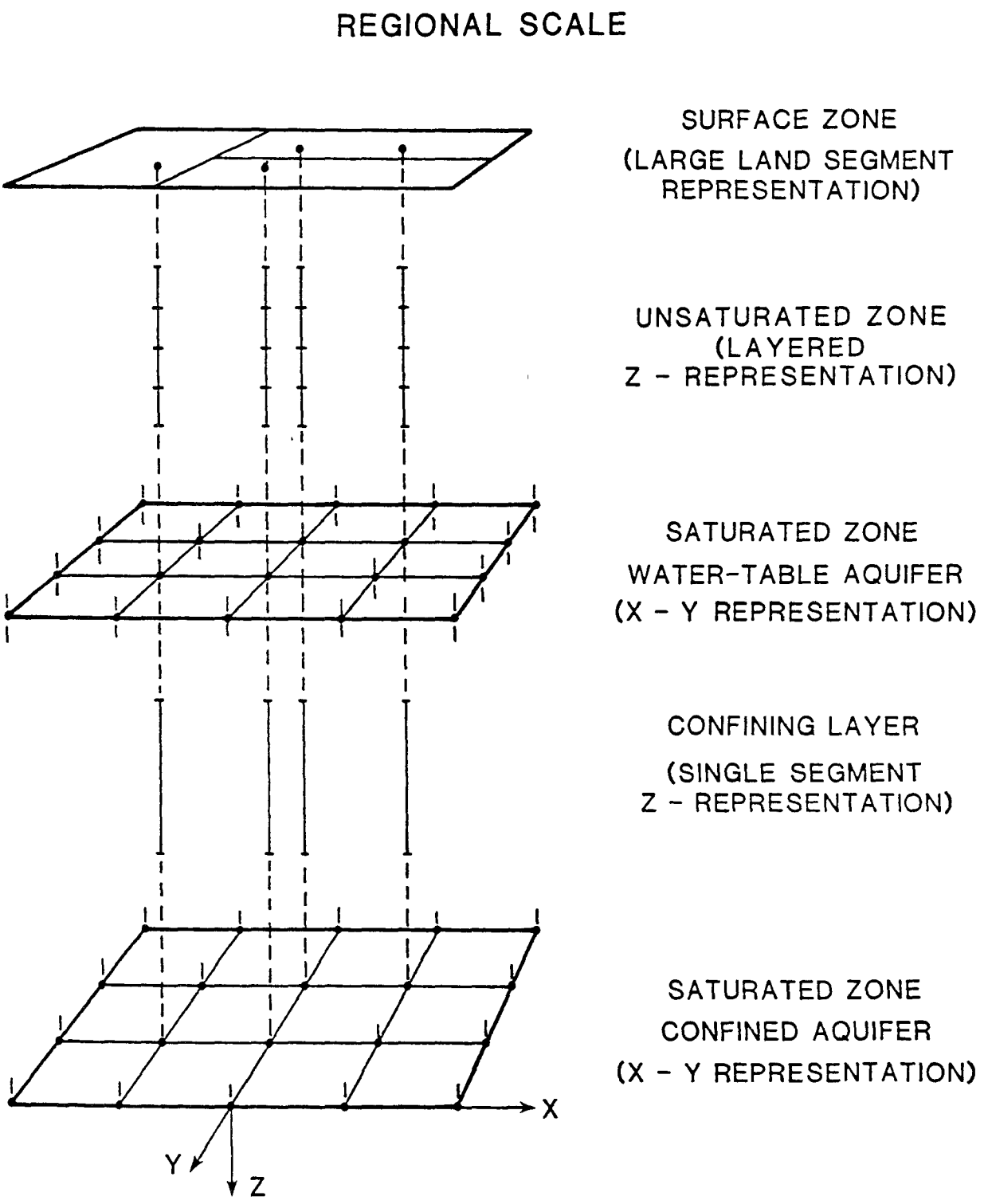


Fig. 9b. Typical dimensionalities used to represent surface unsaturated zones in regional groundwater models (from van der Heijde 1988).

resulting in different approaches in aggregating small scale phenomena into large scale models (Figures 9a,b).

Note the difference in treatment of the vertical components in groundwater models. In the regional models the flow in soils and between aquifers is mainly one-dimensional and vertical, to reduce the computational load. Here, the flow between aquifers is generally represented by a single unit while the flow in soils might be vertically discretized. In the local model, second-order effects may be important enough to warrant the use of two-dimensional vertical or three-dimensional simulation in the soil zone.

Another example can be found in simulating solute transport in fractured porous media where the movement of the solute in the fractures can be two orders of magnitude greater than in the porous matrix. Here, a split-time approach, using different time step sizes for simulating the processes that take place in the fractures and in the porous rock, increases the efficiency of the simulations (DeAngelis et al. 1984).

With the increasing capacity and decreasing cost of computers, a trend prevails toward using smaller time scales for the same types of problems, resulting in higher temporal resolution.

MODEL GRID DESIGN

In the application of numerical models, one of the elements most critical to the accuracy of the computational results is the spatial and temporal discretization chosen. Spatial discretization is represented by the grid overlaying the aquifer and formed by cells (finite-difference method) or elements (finite-element method) defined by interconnected nodes. These cells might be one-, two- or three-dimensional in nature, depending on the dimensionality of the model. The discretization in time is represented by the sequence of time steps selected for the simulation calculations.

Grid Shape and Size

There are various ways to discretize a groundwater system in space, primarily determined by the numerical method chosen. A major distinction exists between the rather rigid grid required by the common finite-difference method and the rather flexible grid allowed by many models based on the finite-element method, and by such modeling approaches as the polygon-based integrated finite-difference method. The option to use two-dimensional triangles and quadrilateral elements and their three-dimensional equivalent in the finite-element method allows the user to deal efficiently with rather irregular geometries. In some finite-element models this flexibility is further enhanced by using internal nodes or so-called "pinch" nodes in selected elements, e.g. to go from areas the grid needs to provide for a high resolution, to areas with a low grid density (Voss 1984).

Additional distinctions exists within the major numerical methods, e.g. between fixed and variable grid spacing in finite-difference grids and between fixed and variable element shape and size in the finite-element method. Other numerical methods might have their own specific requirements, such as the boundary element method with respect to discretization along the boundaries.

The rigid discretization grid for finite-difference models has a major advantage over the flexibility of the finite-element method in that it allows efficient nodal and cell-wise ordering of the set of equations, providing for efficient matrix solution techniques, simple grid design, and relatively easy input data preparation. However, especially in the case of irregular external and internal model boundaries, complex hydrogeologic zone boundaries, etc.. the flexibility of the finite-element method allows the user to select many fewer elements and thus many fewer equations to solve than is needed for a finite-difference solution obtaining the same accuracy in the computational results. To closely follow irregular boundaries using a finite-difference approach requires a rather dense grid, inadvertently resulting in many inactive cells outside the model area being included in the solution procedure. This characteristic difference between the two major numerical modeling approaches is well illustrated by various published modeling studies of the flow system in the Musquodaboit Harbor Aquifer, Nova Scotia, Canada. The first numerical modeling study applied a finite-difference model with a regular square grid having about 2600 nodes (Pinder and Bredehoeft 1968). According to Pinder and Frind (1972) this number of nodes could be reduced to approximately 25% by using a variable finite-difference grid. Pinder and Frind (1972) demonstrated the advantages of the finite-element method by obtaining a close match with the finite-difference prediction in Pinder and Bredehoeft (1968), using only 96 nodes and 44 carefully designed and located deformed isoparametric quadrilateral elements. To reduce the time-consuming design that such an optimal grid requires, Huyakorn (1984) used 195 automatic, computer-generated triangular and rectangular elements in the verification runs of a finite-element flow and transport code. Here, some of the computational efficiency is given up to achieve an economically optimal grid design based on computer and personnel costs for both preparation and performing of the simulation runs.

Design Criteria

Traditionally, designing a grid is a rather intuitive process, increasingly performed with assistance of (semi-)automatic grid generation and interactive computer graphics techniques (Sartori et al. 1982, Drolet 1986). Each grid must be designed for the particular aquifer under study, according to the purpose of the investigation, the quality of data on geometry, properties, and boundary conditions, and cost constraints (Townley and Wilson 1980). A major consideration should be striking a balance between data processing costs (computer, personnel) and required accuracy. Selecting more nodes means solving more equations, which in turn requires more computer memory and computer time.

A number of general principles apply. Among these, the grid should be designed to optimally represent:

- external and internal boundaries such as recharge, no-flow, geologic formation boundaries, and low velocity zones (e.g., liners)
- external and internal stresses such as river stages, wells (both injection and discharge), pollution sources (e.g., point sources versus nonpoint sources), and recharge rates.

Additional considerations include:

- aligning where possible the main grid orientation with the principle direction of flow and transport (or hydraulic parameters, e.g., transmissivity)
- using a fine grid in areas where results are needed, e.g., in the area of highest pollution or highest drawdown
- using a coarse grid where data are scarce or for parts of the model area away from the area of interest
- spacing nodes close together in areas having large changes in transmissivity or hydraulic head, or where concentration gradients are significant
- where possible, let internal and external boundaries coincide with element boundaries
- locate "well" nodes (both active wells and observation wells) near the physical location of the well.

To address the need for a fine grid in areas of interest in a large-scale system, a modeling technique is used based on successive stages of localization of scale and adjustment of grid spacing. This stepwise technique is sometimes referred to as telescoping (Ward et al. 1987). Related to this approach is the use of different scales for simulating the flow part and the transport part, using the same modeling software (Konikow 1985). To fulfill the stringent requirements for flow boundary conditions in local transport simulations, a regional flow model is prepared to provide the required information.

It should be noted that three-dimensional modeling constitutes a significant increase in complexity in comparison with two-dimensional modeling. An important distinction exists between quasi-three-dimensional modeling and fully three-dimensional modeling. In quasi-three-dimensional modeling the grid consists of two-dimensional horizontal grids representing the vertically averaged flow and transport in the individual aquifers connected by a one-dimensional single cell or element representing the connecting aquitards. In fully-three-dimensional modeling the cells or elements can be three-dimensional (but also two- or even one-dimensional as in dual porosity systems; see Chapter 5).

Problems may occur when internal no-flow areas are represented in the model by cells or elements with zero transmissivity value (Townley and Wilson 1980). In such a case, it may be better to create a hole in the grid, a zone internal to the modeled area but not included in the model itself.

It should be noted that in using the finite-element method the solution efficiency depends on node numbering. Modern finite-element codes often include a node and element-numbering optimization routine, especially if automatic grid generation is provided for.

Grid Design and Numerical Accuracy

There is a direct relationship between numerical accuracy and stability, grid density and time step size Huyakorn and Pinder 1983). Numerical accuracy often can be improved by reducing the grid spacing, as the truncation error in the numerical approximations is proportional to $\Delta\ell^2$ (where $\Delta\ell$ is grid spacing). A related numerical problem is the occurrence of oscillations. Various methods exist to reduce this problem, such as using the Peclet number

$$P_e = v \cdot (\Delta t) / D < 2$$

in reducing grid spacing, or modifying the time step to conform to the Courant criterion

$$C_r = v \cdot (\Delta t)/(\Delta\ell) \leq 1$$

Oscillations can also be reduced by using spatial or upstream weighting.

To reduce numerical problems when variable grid spacing is present, the changes in size between neighboring cells or elements should be restricted. For instance, as a rule-of-thumb in using a finite-difference model, the grid may be expanded toward distant boundaries by a factor 1.5 to 2. Likewise, in using a finite-element model, triangular elements should be kept as equilateral as possible. Elements with a length-to-width ratio of more than five tend to give poor accuracy results (Townley and Wilson 1980). The presence of anisotropy can further restrict this ratio. Another finite-element condition frequently required to avoid numerical problems limits the size difference between neighboring elements to less than a factor of five (Townley and Wilson 1980).

Often, in solving non-steady-state problems, one of three finite-difference approximations for the time variable is used: explicit, fully implicit, and Crank-Nicolson schemes (Huyakorn and Pinder 1983). If the explicit method is used, a stability criterion applies, dependent on the type of differential equation solved and the numerical method used. Such a criterion specifies the maximum value for the time step to avoid uncontrolled growth of the numerical error during the solution process. The other two time approximation methods are unconditionally stable.

In simulating multiphase flow using certain five-point finite-difference approximations (as in a grid with rectangular or square cells: center node and four surrounding nodes), a numerical difficulty often described as "grid orientation effect" occurs. The results of computations with a grid diagonal to the principal direction of fluid movement may be quite different from those with a parallel grid, both being significant in error with the real answer (Huyakorn and Pinder 1983). Using very refined grids does not reduce the effects of this problem, as the severity of these effects is a direct result of the mobility ratio of the two fluid phases. The solution to this kind of problem is found by using higher-order finite-difference approximations (e.g., nine-point methods), or selecting another solution method such as certain finite-element schemes.

MODEL CALIBRATION

Model calibration is aimed at demonstrating that predictions made with the model are realistic and to a certain extent "accurate" and "reliable" (Konikow and Patten 1985). In addition, calibration is often used to obtain values for parameters that have not been measured or for which no reliable (field) measurement technique is currently available. The iterative process of matching calculated values with observed (historical) data by adjusting model input can take the form of a manual trial-and-error procedure or an automatized procedure (Figure 10). The calibration process is also known as history matching and is closely related to parameter estimation. The result of this process might be in the form of a refinement of initial estimates of aquifer properties (parameters), the establishment of the location of the boundaries (areal and vertical extent of aquifer), and the determination of flow and transport conditions at the boundaries (boundary conditions). Trial-and-error calibration is a highly subjective, intuitive procedure. As data quantity and quality is often limited, no unique set of parameters result, leaving the modeler with a subjective choice. Completion of the calibration process depends on many factors, including the objectives for analysis, the complexity of the groundwater system being studied, the length of the observed history, the accuracy required in the prediction stage, the available budget, the expertise of the modeler, and the patience of the modeler (or the manager waiting for answers).

Automatic calibration procedures are based on the use of prescribed algorithms, their completion achieved when preset matching criteria are met. Because of the formal approach taken in adjusting model input, automatic procedures are less subjective than trial-and-error procedures. In addition, they require fewer computer runs and are also more efficient with respect to staff time required for model output analysis. However, they require the modeler to be well trained in the use of numerical and statistical techniques.

THE ROLE OF SOFTWARE; STAGES OF DATA PROCESSING

The core of the modeling process is the computer-based simulation of the behavior of the groundwater system for a particular management scenario. From the computer software point of view, the simulation is preceded by data acquisition, inspection and storage, data interpretation, and model input preparation (Figure 11). This data-processing stage is often called (simulation-) preprocessing. Post-processing involves storage, analysis, and presentation of the computational results (van der Heijde and Srinivasan 1983). Computer-based numerical interpolation and statistical techniques as well as graphical methods might be employed in the pre- and postprocessing stages.

Field data acquisition can be either manual or computer driven. In the latter case it is often combined with various data handling techniques. Transfer of data collected in the field to computer-based storage facilities can be indirect, using data sheets and analog registration and manual computer data entry, or directly by measurement-linked, on-site storage of data on magnetic media or by immediate electronic transfer from a measurement device to remote storage facilities, often a remote-controlled process. The initial data storage of unprocessed field data must be followed by data checking and screening for measurement and transmission errors, after which they are stored as conditioned data.

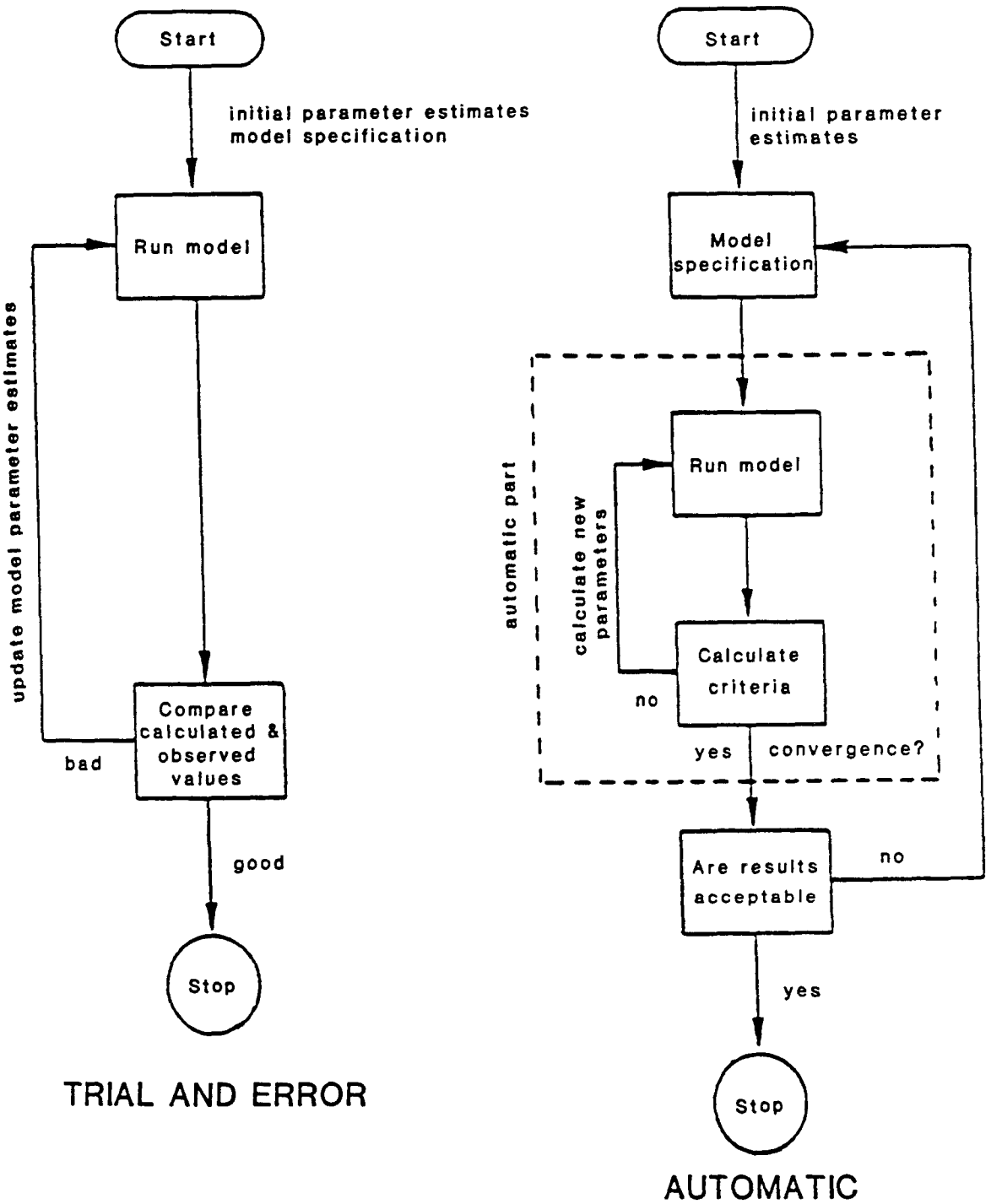


Fig. 10. History matching/calibaration using trial and error and automatic procedures (after Mercer and Faust 1981).

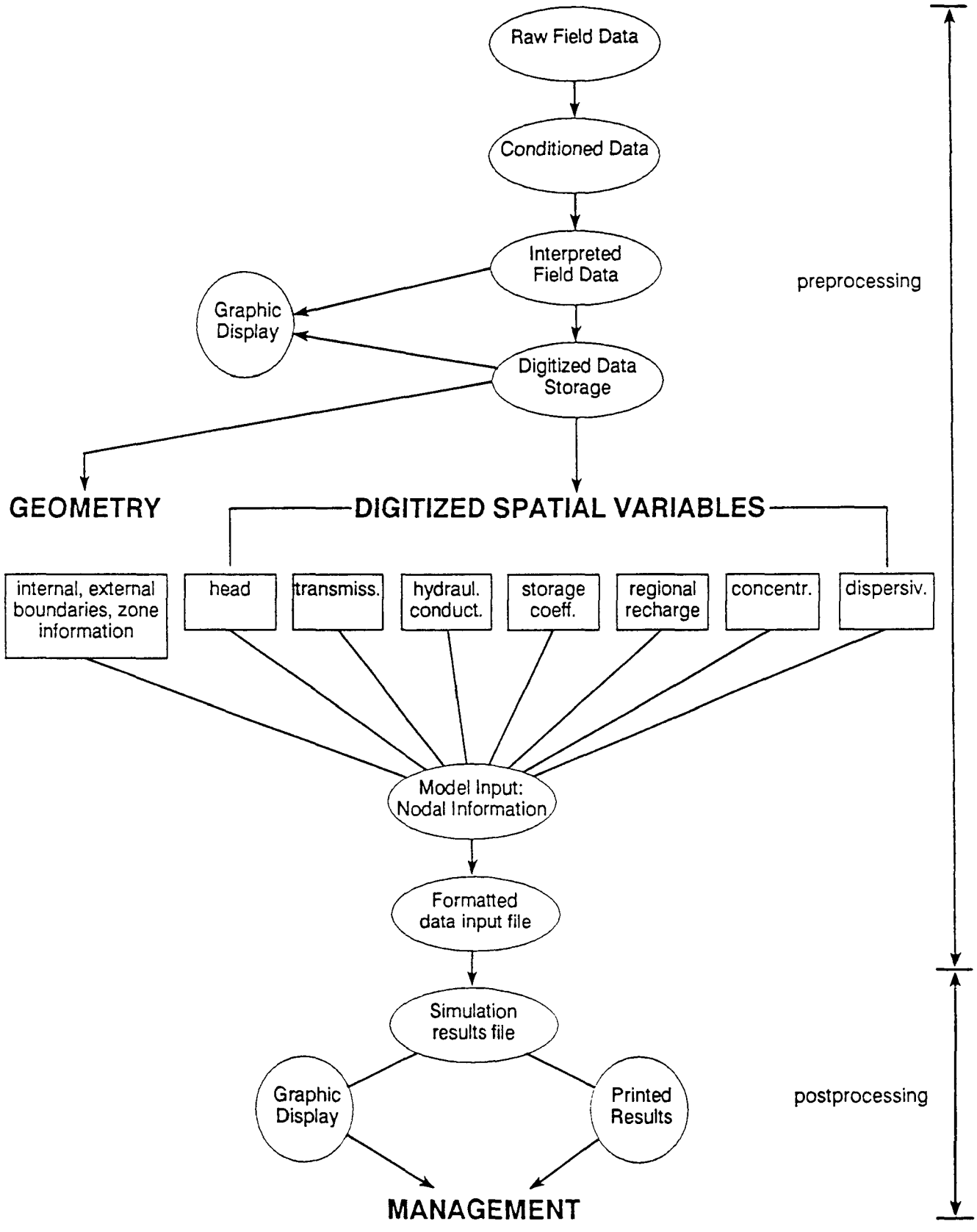


Fig. 11. Decision-support data stream in modeling.

Interpretation of field data results in an information set on the system studied, again stored for further use. The next step is the model gridding followed by nodal or elemental assignment of model input parameters. This step often requires further interpretation or at least, interpolation of available data. After appropriate formatting the preprocessing stage is finished and the simulation runs can start. Many steps in the preprocessing stage can be computerized. This is especially true for such data handling activities as error-checking, reformatting, and storing. However, automation should not limit the modeler's ability to intervene in each stage of the modeling process.

The simulation program can be run in a batch mode, requiring user-specified input files. In such a case the model runs independently of any direct user interaction. A user-prepared file, a so-called batch file containing a sequence of computer operating system instructions, drives the program execution. If the user has the option to interact with the program during its execution, modeling becomes more flexible. Such interaction might facilitate changing stresses during successive simulation steps, changing such modeling variables as timestep sequences, or even changing values for system parameters. The most common user interaction is a restart option provided by some software where the latest computed values for the dependent variable are used as initial values for the new run.

If preprocessing is combined with simulation, three approaches are possible (Figure 12). First, data can be entered directly into a file from prepared data sheets, using a generic program such as a word processor or line editor, followed by a "batch run" of the code, a process in which no user interaction with the computer is allowed during code execution. The user needs to ensure that the data formats required by the simulation program are correctly applied. The second approach uses a dedicated computer program facilitating interactive data entry, data formatting and storing, followed by a batch run of the code. Finally, data can be entered interactively, guided by the same program that contains the simulation algorithms. Some programs based on this latter approach allow the user to influence program execution during the simulation runs.

In the interactive use of a computer, a program directs the interaction between user and computer. The user selects a continuation option at each decision point in the program. Increasingly, the user might be assisted at the various decision-making points by expert systems providing decision-making logic, data options, error-checking, and report facilities.

In using a numerical model, input data preparation is a time-consuming activity. The user who is unfamiliar with the format specifications of the model will make many mistakes during data entry: format errors, incorrect data sequences, and others. Interactive data entry with a dedicated preprocessor is especially advantageous for a user who is relatively inexperienced in data formatting, file handling, and running simulation software in general. Furthermore, preprocessors are often used in local preparation of the input files for remote computers.

The postprocessing stage includes a variety of data-handling activities. Computational results are routed to mass-storage devices such as disk drives, displayed on a video screen or printed (Figure 12). They can be used in

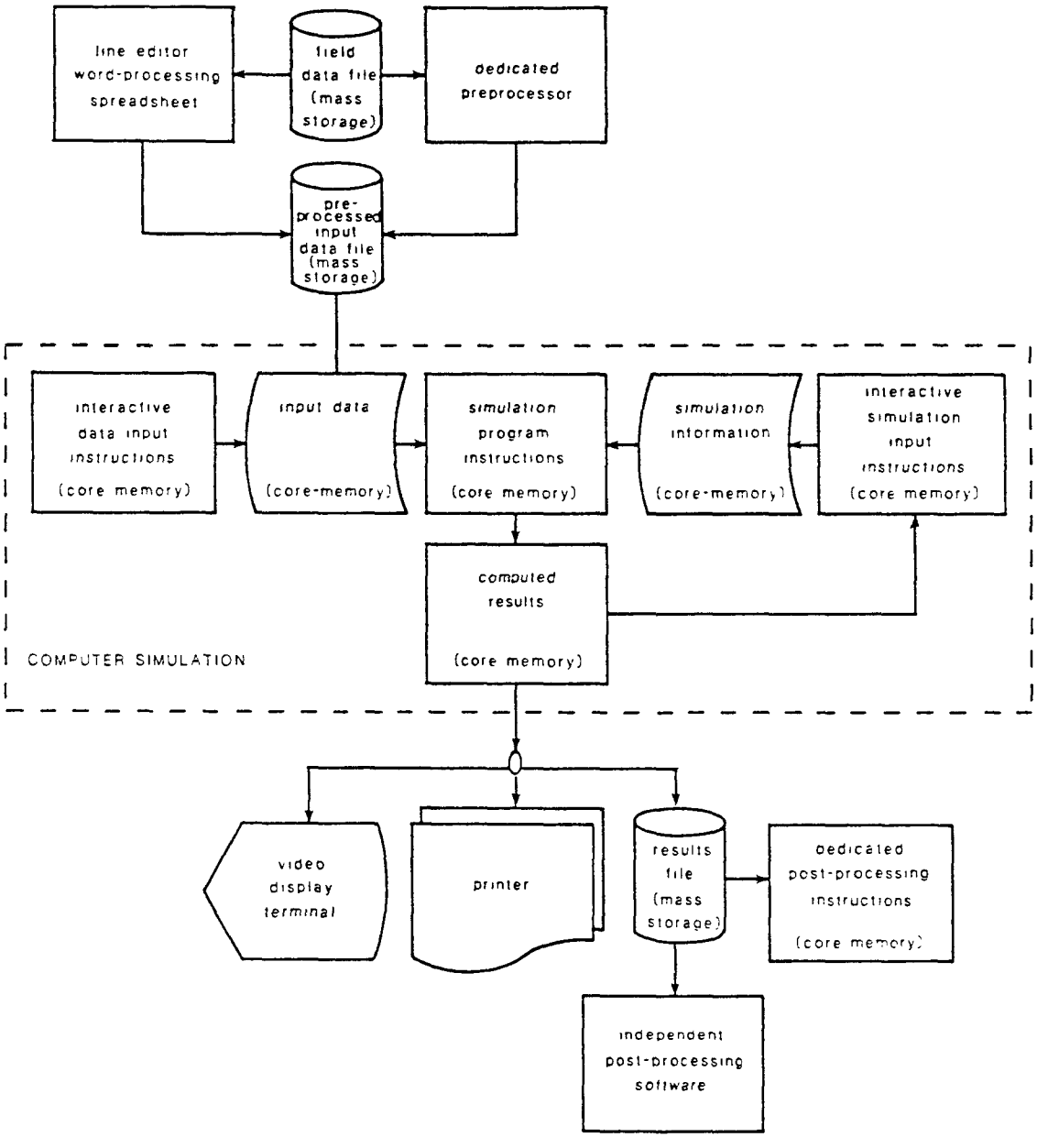


Fig. 12. Data preparation and code execution.

subsequent programs for postsimulation analysis or graphic presentation using a screen terminal or plotter.

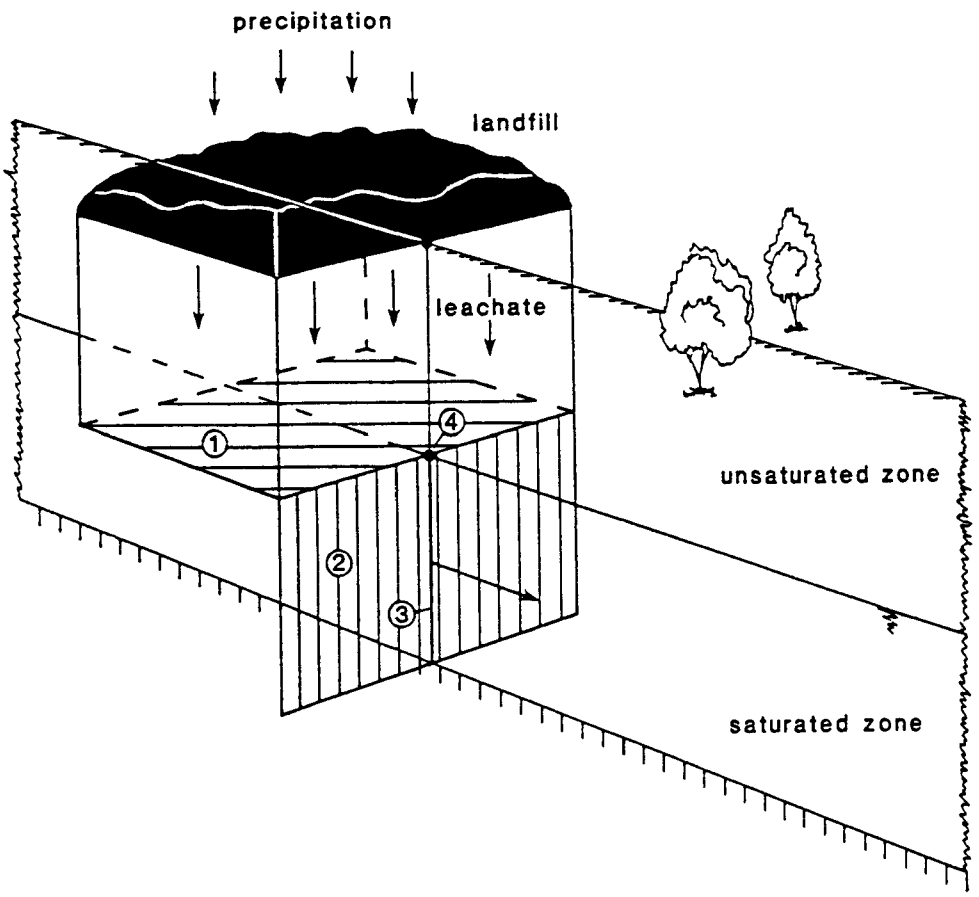
Postprocessors might be used to reformat and display or print the results in textual or graphic form and to analyze the results by means of a variety of manual and automated techniques (van der Heijde and Srinivasan 1983). For most models, output for graphic display such as contouring can be obtained by processing one of the output files directly, using display software, or after some simple modifications in the simulation code. If the software does not already have the option to generate time drawdown curves for selected locations, the code itself has to be changed to facilitate this feature, a requirement that might not be easily met in the microcomputer environment. However, this kind of problems are expected to decrease with the next generation of microcomputers and microcomputer operating systems and new application software. Display of streamlines and isochrones, among others, requires dedicated software, coupling simulation, and graphics software. Information on graphic pre- and postprocessing software can be found in Beljin (1985), among others.

A special form of computerized data processing is provided by computer graphics. Computer graphics consists of a combination of data structures, graphic algorithms, and programming languages. The use of graphics is helpful in presenting information and facilitates the visual inspection and analysis of certain data structures (e.g., spatial hydrogeologic characteristics and spatial and temporal distributions of computed results.) Until recently, computer graphics was mainly used to display the results of a simulation. Recent developments in computer technology have made it possible to digitize large volumes of mapped data and to use graphics interactively in the design stage of a model. Generic software such as CAD/CAM programs (Computer Aided Design/Computer Aided Manufacturing) or dedicated graphic software are increasingly used for such tasks as the development or alteration of model grids. Coupled with dedicated software, the digitized data can be automatically transformed into grid-based model input, using interpolation algorithms and reformatting techniques. Thusfar, these developments have been introduced in experimental projects (e.g., Fedra and Loucks, 1985) and some proprietary software (e.g., Kjaran et al. 1986). Currently some of these concepts are included in software developments projects (P. Bedient, Rice University, Houston, pers. comm., and C. Cole, Battelle PNL, Richland, WA, pers. comm.)

MODELING SOURCES OF GROUNDWATER POLLUTION

In modeling sources of groundwater pollution, the source must be described in terms of its spatial, chemical, and physical characteristics, and its temporal behavior. The spatial definition of the source includes location, depth, and areal extent, and together with the scale of modeling identifies the source as a point source, a line source, a distributed source of limited areal or three-dimensional extent, or as a nonpoint source of unlimited extent (van der Heijde 1986). Figure 13 shows the effect of different ways of modeling the leachate of a landfill entering an aquifer as boundary condition on the spreading of a plume in the aquifer. Both the areal and vertical extent of the plume are influenced by the choice of the spatial dimensions of the source. Furthermore, the areal extent of the source in relation to the scale of modeling determines the spatial character of the

a. various ways to represent source.



b. horizontal spreading resulting from various source assumptions.

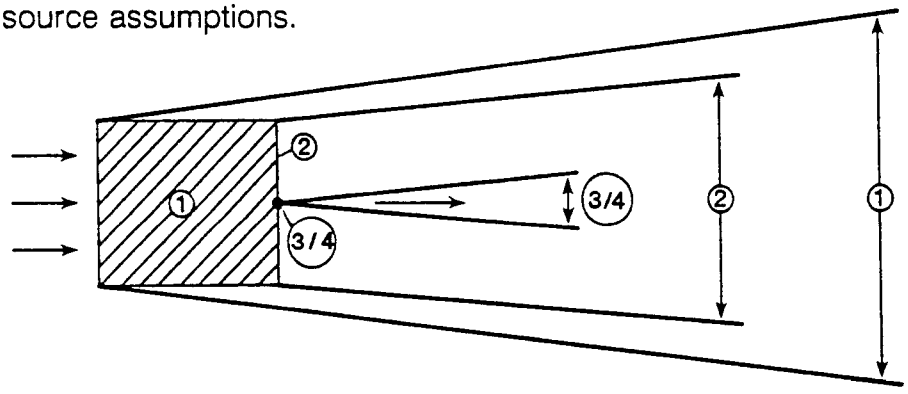
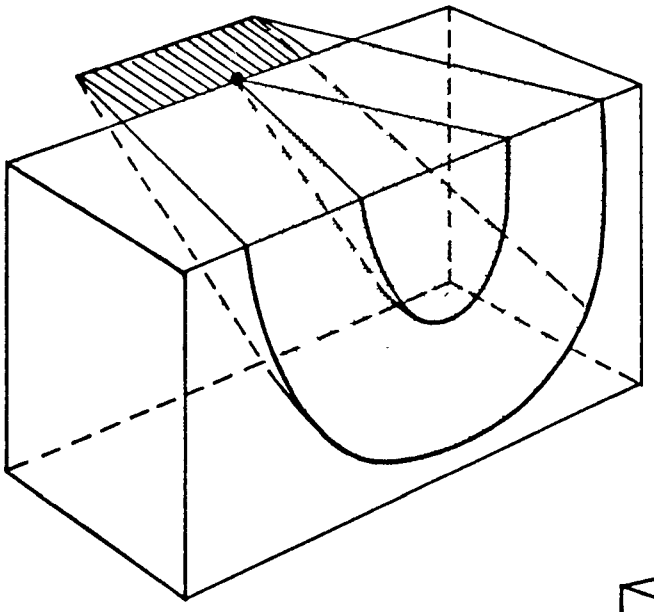
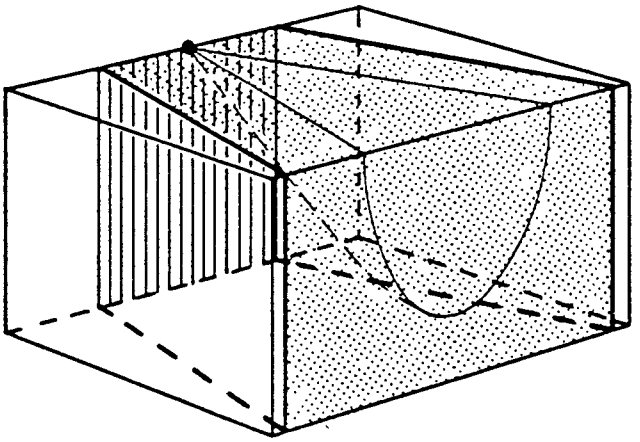


Fig. 13. Definition of the source boundary condition under a leaking landfill (numbers 1....4 refer to case 1....4).

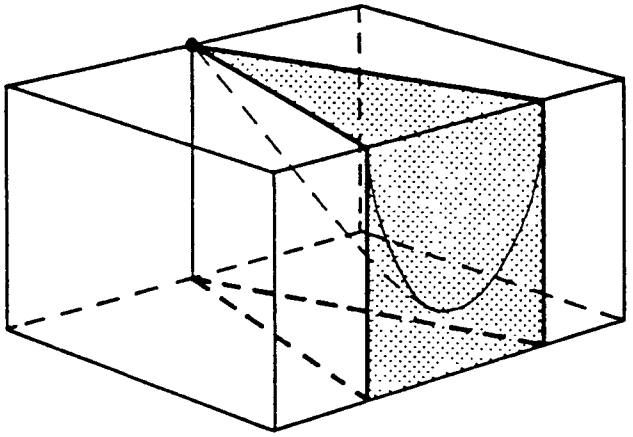
c. detailed view of 3D spreading for various ways to represent source boundary.



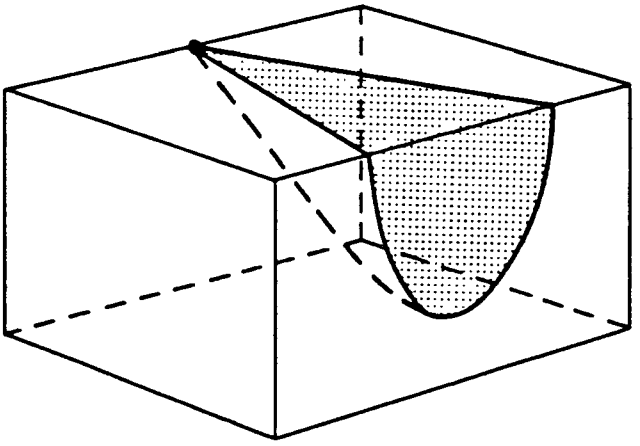
Case 1:
horizontal 2D-areal source at top of aquifer (for 3D modeling)



Case 2: vertical 2D-source in aquifer (for 2D horizontal, vertically averaged, or 3D modeling)



Case 3:
1D vertical line source in aquifer (for 2D horizontal, vertically averaged, 2D cross-sectional, or 3D modeling)



Case 4: point source at top of aquifer (for 2D or 3D modeling)

Fig. 13 (continued).

source in the model. In some cases a nonpoint pollution source for a local scale model is considered a point pollution source for modeling at a regional scale (e.g., septic tanks, landfills, feedlots).

The source can be located at the boundary or within the system for which the model is developed. In this respect, the choice of system boundaries is important: a source located in the unsaturated zone is an internal source for a model that includes this zone, but is a boundary source for a model of the saturated zone alone. Not only are different types of models required (variably saturated versus saturated zone models), but the models need to facilitate the source in different mathematical ways, i.e., as an internal source or as a boundary condition, respectively. An overview of the source types and their spatial characteristics for modeling is presented in Table 3 (van der Heijde 1986).

Another source characteristic important to the modeling process is its history or expected behavior in time. The source can be continuous in time, either fluctuating or constant in strength (e.g., landfills, impoundments, feedlots), or in the form of a pulse or series of individual, non-overlapping pulses (e.g., spills, leaching of agrochemicals during or after a storm).

A conceptual difficulty is that of incorporating the effect of the unsaturated zone on the concentration and arrival time of contaminants reaching the groundwater. The heterogeneity of this zone, and the complex transformations that occur in this soil-plant-water-air environment, contribute to this difficulty.

In certain cases, modeling may be used to trace the source of an existing pollution plume. For convection-dominated transport, this can be done directly. However, the irreversibility of some of the chemical and physical processes (e.g., dispersion) necessitates the use of models for this problem in an indirect manner. Here, an iterative approach assumes a certain source in space and time and a certain strength, and predicts the current position of the plume.

MODELING WASTE DISPOSAL FACILITIES, PROTECTION AREAS, MONITORING NETWORKS, AND REMEDIAL ACTIONS

Models are used increasingly in evaluating designs for controlled waste management facilities. Many engineering designs for such facilities are also useful for restoring a contaminated groundwater system. To this purpose various technologies have been developed. Restoration or remedial action technologies can be classified into three groups: surface controls, subsurface controls, and waste controls (JRB Associates 1982) (see Table 3). In addition, models can provide guidance in designing the pollution monitoring systems required by federal, state, and local regulations.

To use modeling of designed-system alterations and remedial action for evaluation of performance and efficiency, aspects such as model type and dimensionality, grid configuration, system stresses and constraints, and parameter adjustments, are important (Boutwell et al. 1985). Table 4 provides an overview of modeling aspects of various engineering activities and remedial actions in groundwater systems. For each design feature, the effects on the

Table 3. Sources of groundwater pollution and model representations (from van der Heijde 1986).

Sources	Representation in model
Waste disposal	
Solid waste	
type:	
household, commercial, and industrial waste	
sludge from water-treatment plants and air-pollution control facilities	
mine tailings	
disposal facilities	point surface or areal surface source
uncontrolled dumps	or point or 3-D near-surface source
sanitary and secured landfills	
deep-subsurface burial (e.g., high-level radioactive waste)	point or 3-D internal source
Liquid waste	
type:	
domestic, municipal and industrial waste water	
disposal facilities:	
wastewater impoundments	point or areal surface source
deep-subsurface injection	point or vertical internal line source
land spraying	nonpoint surface source
discharge in surface water bodies	line or areal surface source
individual sewage disposal systems	point or nonpoint surface or near-surface source
Accidental spills or unforseen leakage	
leachate of solid waste	same as for solid waste
leakage from:	
surface storage facilities (e.g., impoundments)	point or areal surface source
subsurface storage facilities (e.g., gasoline tanks)	point or areal near-surface source
subsurface transport systems (e.g., sewers, pipelines)	near-surface or internal line source
subsurface disposal facilities (e.g., deep well injection)	point-internal or vertical line-internal source
surface spills	point or areal surface source

Table 3. (continued)

Sources	Representation in model
Agricultural pollution	
application of chemicals (fertilizers, herbicides, pesticides)	nonpoint surface source
production of manure (feedlots, intensively used rangelands)	point or areal surface source
irrigation with polluted or saline water	areal or nonpoint surface source
Radioactive waste	
radiological toxicity or both radiological and chemical	same as for solid and liquid waste
solid, liquid, or gaseous radioactive components	
high- or low-level waste, with different ways of controlled disposal	
accidental releases	point or areal surface source
Other sources	
highway deicing salts	line surface source
mobilization of heavy metals in soil by acid rain	nonpoint near-surface source
infiltration of polluted surface water	areal (lake) or line (river) surface source
saltwater intrusion or upconing	boundary source or internal source

Table 4. Modeling designed-system alterations and corrective action (after Boutwell et al. 1985).

Design Feature	Effects on Groundwater
Capping, grading, and revegetation	Reduction of infiltration
	Reduction of successive leachage generation
Groundwater pumping (and optional reinjection of treated water)	Changes in heads, direction of flow, and contaminant migration
	Controlled plume removal
Wastewater injection	Changes in heads and direction of flow
	Plume generation
Interceptor trenches	Changes in heads, direction of flow, and contaminant migration
	Plume removal
Impermeable barrier (optional drainage system to prevent mounding)	Containment of polluted water
	Routing unpolluted groundwater around site
	Changes in heads and direction of flow
Subsurface drains	Removal of leachate
	Changes in heads, direction of flow, and contaminant migration
Solution mining	Removal of contaminants after induced mobilization
Excavation	Removal of waste material and polluted soil
	Changes in hydraulic characteristics and boundary conditions
	Changes in heads and direction of flow

Table 4. (continued)

Design Feature	Type of Model Required
Capping, grading, and revegetation	Unsaturated zone model, vertical layered
Groundwater pumping (and optional reinjection of treated water	Saturated zone model, two-dimensional areal, axisymmetric or three-dimensional; Well or series of wells assigned to individual node
Wastewater injection	Saturated zone model, two-dimensional area, axisymmetric or three-dimensional; Density-dependent flow; Temperature difference effects
Interceptor trenches	Saturated zone model, two-dimensional areal or cross-sectional, or three-dimensional; Trenches are represented by line of notes with assigned heads
Impermeable barrier (optional drainage system to prevent mounding)	Saturated zone model, two-dimensional areal or cross-sectional, or three-dimensional; possibly two-dimensional cross-sectional unsaturated zone model for liners
Subsurface drains	Saturated or combined unsaturated-saturated zone model, two-dimensional cross-sectional or three-dimensional
Solution mining	Saturated or combined unsaturated-saturated zone model, two-dimensional areal, cross-sectional or three-dimensional; Lines of sources (injection) and sinks (removal)
Excavation	Unsaturated, saturated, or combined unsaturated-saturated zone model; for unsaturated some model minimal one-dimensional vertical, for other types minimal two-dimensional, cross-sectional

Table 4. (continued)

Design Feature	Typical Modeling Problems
Capping, grading, and revegetation	Parameters related to leaching characteristics of reworked soil
Groundwater pumping (and optional reinjection of treated water)	Representing partial penetration
Wastewater injection	Representing density-dependent effects
Interceptor trenches	Representing partial penetration, resolution near trenches
Impermeable barrier liners (optional drainage systems to prevent mounding)	Representing partial penetration, flow and transport around end of barrier(s)
	Conductivity liner or barrier material
	Large changes in conductivity between neighboring elements
	Differences in required grid resolution
Subsurface drains	Resolution near drain
Solution mining	Parameters related to mobilization (sorption coefficient, retardation coefficient)
Excavation	Parameters of backfill material

groundwater system, model requirements, and specific modeling problems are listed.

The selection of the type of model depends on whether surface water, unsaturated zone, or saturated zone systems are to be modeled, or a combination thereof. In groundwater, each situation is three-dimensional. However, processes in two directions may be orders of magnitude larger than in the third direction; then, areal or cross-sectional two-dimensional modeling is justifiable. Grid configuration reflects spatial characteristics of source, plume, and designed actions. The engineered modifications may require parameter adjustments and adjustments of the boundary conditions.

In remedial action modeling one is often confronted with data lacking on the following aquifer characteristics:

- In-place hydraulic conductivities for different impermeable barrier materials
- Changes in chemical mobility caused by injection of chemicals and solution mining
- Hydraulic properties and sorption characteristics of permeable treatment beds
- Changes in chemical susceptibility to degradation resulting from bioreclamation
- Alteration of properties by chemical interaction with the barriers.

Other problems encountered that are typical for modeling of remediation alternatives include code limitations on gridding flexibility, numerical problems in zones with high-contrast soil or rock properties (heterogeneity), and inaccuracies where the flow field changes significantly in velocity and direction (see Table 4). For a more in-depth discussion of these issues see Boutwell et al. (1985).

5. MODEL OVERVIEW

TYPES OF MODELS

Groundwater models can be divided into various categories, depending on the purpose of the model and how the nature of the groundwater system is described. Apart from spatial resolution (one, two, or three dimensions), and temporal definition (steady-state flow or transport versus time-dependent behavior), models can be distinguished by the process they are designed to simulate (van der Heijde et al. 1985a).

Flow models simulate the movement of one or more fluids in porous or fractured rock. One such fluid is water; the others, if present, can be air (in soil) or immiscible nonaqueous phase liquids (NAPLs) such as certain hydrocarbons. A special case of multifluid flow occurs when layers of water of distinct density are separated by a relatively small transition zone, a situation often encountered when sea water intrusion occurs. Flow models are used to calculate changes in the distribution of hydraulic head or fluid pressure, drawdowns, rate and direction of flow (e.g., determination of streamlines, particle pathways, velocities, and fluxes), travel times, and the position of interfaces between immiscible fluids (Mercer and Faust 1981, Wang and Anderson 1982, Kinzelbach 1986, Bear and Verruijt 1987).

Two types of models can be used to evaluate the chemical quality of groundwater (e.g., Jennings et al. 1982, Rubin 1983, Konikow and Grove 1984, Kincaid et al. 1984): (1) pollutant transformation and degradation models, where the chemical and microbial processes are posed independent of the movement of the pollutants; and (2) solute transport models simulating displacement of the pollutants, often including the effects of transformation and degradation processes (transport and fate).

Hydrochemical models represent the first type, as they consist solely of a mathematical description of equilibrium reactions or reaction kinetics (Jenne 1981, Rice 1986). These models, which are general in nature and are used for both groundwater and surface water, simulate chemical processes that regulate the concentration of dissolved constituents. They can be used to identify the effects of temperature, speciation, sorption, and solubility on the concentrations of dissolved constituents (Jenne 1981).

Solute transport models are used to predict movement, concentrations, and mass balance components of water-soluble constituents, and to calculate radiological doses of soluble radionuclides. A solute transport model uses the (piezometric) head data generated by a flow model to generate velocities for advective displacement of the contaminant, allowing for additional spreading through dispersion (Anderson 1984) and for transformations by chemical and microbial reactions. The transformations considered by so-called nonconservative models are primarily adsorption, radioactive decay, and biochemical transformations and decay (Cherry et al. 1984, Grove and Stollenwerk 1987).

The inclusion of geochemistry in solute transport models is often based on the assumption that the reaction rates are limited and thus depend on the residence time for the contaminant, or that the reactions proceed instantaneously to equilibrium. Recently, various researchers have become inter-

ested in a more rigid, kinetic approach to incorporate chemical reactions in transport models (e.g., Bahr and Rubin 1987). This inclusion of geochemistry has focused on single reactions such as ion-exchange or sorption for a small number of reacting solutes (Rubin and James 1973, Valochi et al. 1981, Charbeneau 1981). Because multicomponent solutions are involved in most contamination cases, there is a need for models that incorporate the significant chemical interactions and processes that influence the transport and fate of the contaminating chemicals (Cederberg et al. 1985). This is especially important in simulating fate and transport of mixed wastes.

In some cases, comprehensive groundwater quality assessment requires the simulation of temperature variations and their effects on groundwater flow and pollutant transport and fate. A few highly specialized multipurpose prediction models can handle combinations of heat and solute transport, or either heat transport or solute transport together with rock matrix displacement (P. Huyakorn, Hydrogeologic, Inc.; B. Sagar, Rockwell International, Inc.; pers. comm.). Generally, these models solve the system equations in a coupled fashion to provide for analysis of complex interactions among the various physical, chemical, and biological processes involved. None of these models has yet been released for general use.

As groundwater is part of a larger physical system, the hydrologic cycle, many models address in one way or another the interaction between groundwater and the other components of the hydrologic cycle. Some of these models describe only the interactions, sometimes as a process, sometimes as a dynamic stress or boundary condition. Increasingly, models are developed that simulate the processes in each subsystem in detail, in addition to the interrelationships (e.g., Morel-Seytoux and Restrepo 1985). Two types of models fit this latter category: watershed models and stream-aquifer models (sometimes called conjunctive use models).

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

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

For conjunctive use evaluation, models must simulate more processes than those included in watershed models. Important processes to consider include canal seepage, deep percolation from irrigated lands, aquifer withdrawal by pumping, groundwater inflow to or outflow from adjacent aquifers, plant transpiration, artificial recharge, bank storage effects, and deep-well injection (El-Kadi 1986). The inclusion of detailed groundwater flow processes in

watershed models increases significantly the complexity of model computations. Differences in temporal scale between surface and subsurface processes add to the complexities.

Recent interest in such multisystem modeling has increased, motivated by the need to simulate nonpoint pollutant transport such as caused by the widespread use of agricultural chemicals, and by the need to study the contribution of local soil and groundwater pollution to the quality of surface water bodies. To model this type of problem, highly detailed descriptions of transport and fate processes are added to the multisystem flow models.

As management is using a multitude of decision criteria to assure the optimal use of water resources, advanced hierarchical and optimization modeling of surface and subsurface water resources has been of interest to researchers for several years in support of management's decision-making (Haimes 1977).

An overview of watershed models having a significant watershed component is given in El-Kadi (1986). An overview of management models for conjunctive use is presented in van der Heijde et al. (1985a).

The flow and solute transport models may be embedded in a management model describing the system in terms of objective function(s) and constraints, and solving the resulting equations through an optimization technique such as linear programming (Gorelick 1983, Gorelick et al. 1983, Kaunas and Haimes 1985, Wagner and Gorelick 1987).

As an update of van der Heijde (1984) and van der Heijde et al. (1985a) the following sections describe in some detail the mathematical basis of flow and solute transport models and give an overview of the availability and usability of existing flow and solute transport simulation codes. Appendix A through G provide a detailed overview of the most prominent simulation codes currently available.

Several new developments are occurring in groundwater modeling. From the tables in the Appendices it is evident that recently groundwater flow models have evolved to a point where a wide range of flow characterizations are possible. These newer models may include options for various types of boundary conditions as well as the ability to handle a wide variety of hydrologic processes such as evapotranspiration, stream-aquifer exchanges, spatial and temporal variations in recharge, and the more complex characterization necessary for simulating unsaturated flow. Similarly, recently developed models for simulation of solute transport or new versions of earlier models often include increased flexibility in describing the solute source and simulating transport and fate processes such as radioactive decay or chemical transformation and effects of both equilibrium and nonequilibrium adsorption. In some instances, these transport models are coupled with existing geochemical models to provide a more complete analysis of the solute chemistry. Such a development is also noticeable with respect to the simulation of biodegradation, e.g., for the analysis of bioremediation schemes (Borden and Bedient 1986, Borden et al. 1986). Furthermore, important developments have occurred in the modeling of flow and transport in fractured rock systems. Here, both improved site characterization and stochastic analysis of fracture geometry, together with an improved capability to

describe the interactions of chemicals between the active and passive fluid phases and the rock matrix, have facilitated increasingly realistic simulation of real-world fractured rock systems. Multiphase flow models have become increasingly available, especially those designed for studying the movement of immiscible fluids such as NAPLs. Also, new approaches have been developed for parameter identification and are increasingly used in practical applications (Yeh 1986). Finally, optimization-based management models have been applied to a growing variety of decision problems, especially in the area of groundwater protection (Wagner and Gorelick 1987). For the purpose of this review, we consider predictive simulation models that address the processes that comprise groundwater flow, solute, and heat transport, geochemical interactions, and flow and transport in fractured media. Other important types of models such as those describing multiphase flow (e.g., immiscible hydrocarbons, salt water intrusion), automatic parameter identification, and flow and solute transport models coupled with optimization techniques (management models), will be the focus of future evaluation by the IGWMC.

MODEL MATHEMATICS

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

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

Most mathematical models used in groundwater management are distributed-parameter models, either deterministic or stochastic. Their mathematical framework consists of one or more partial differential equations called field or governing equations, as well as initial and boundary conditions and solution procedures (Bear 1979). Models that adopt the stochastic approach assume that the processes active in the system are stochastic in nature and that the variables may be described by probability distributions. Consequently, system responses are characterized by statistical distributions estimated by solving the governing equation.

The governing equations for groundwater systems are usually solved either analytically or numerically. Analytical models contain a closed-form or analytical solution of the field equations, continuous in space and time. An important attribute of analytical solutions is the implicit conservation of

mass (continuity principle). As analytical solutions generally are available only for relatively simple mathematical problems, using them to solve groundwater problems requires extensive simplifying assumptions regarding the nature of the groundwater system, its geometry, and external stresses (Walton 1984, van Genuchten and Alvas 1982).

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

Various numerical solution techniques are used in groundwater models. They include finite-difference methods (FD), integral finite-difference methods (IFDM), Galerkin and variational finite-element methods (FE), collocation methods, boundary (integral) element methods (BIEM or BEM), particle mass tracking methods (e.g., random walk [RW]), and the method of characteristics (MOC) (Huyakorn and Pinder 1983, Kinzelbach 1986). Among the most used approaches are finite-difference and finite-element techniques. In the finite-difference approach a solution is obtained by approximating the derivitaves of the PDE. In the finite-element approach an integral equation is formulated first, followed by the numerical evaluation of the integrals over the discretized flow or transport domain. The formulation of the solution in each approach results in a set of algebraic equations which are then solved using direct or iterative matrix methods (Figure 14).

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

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

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

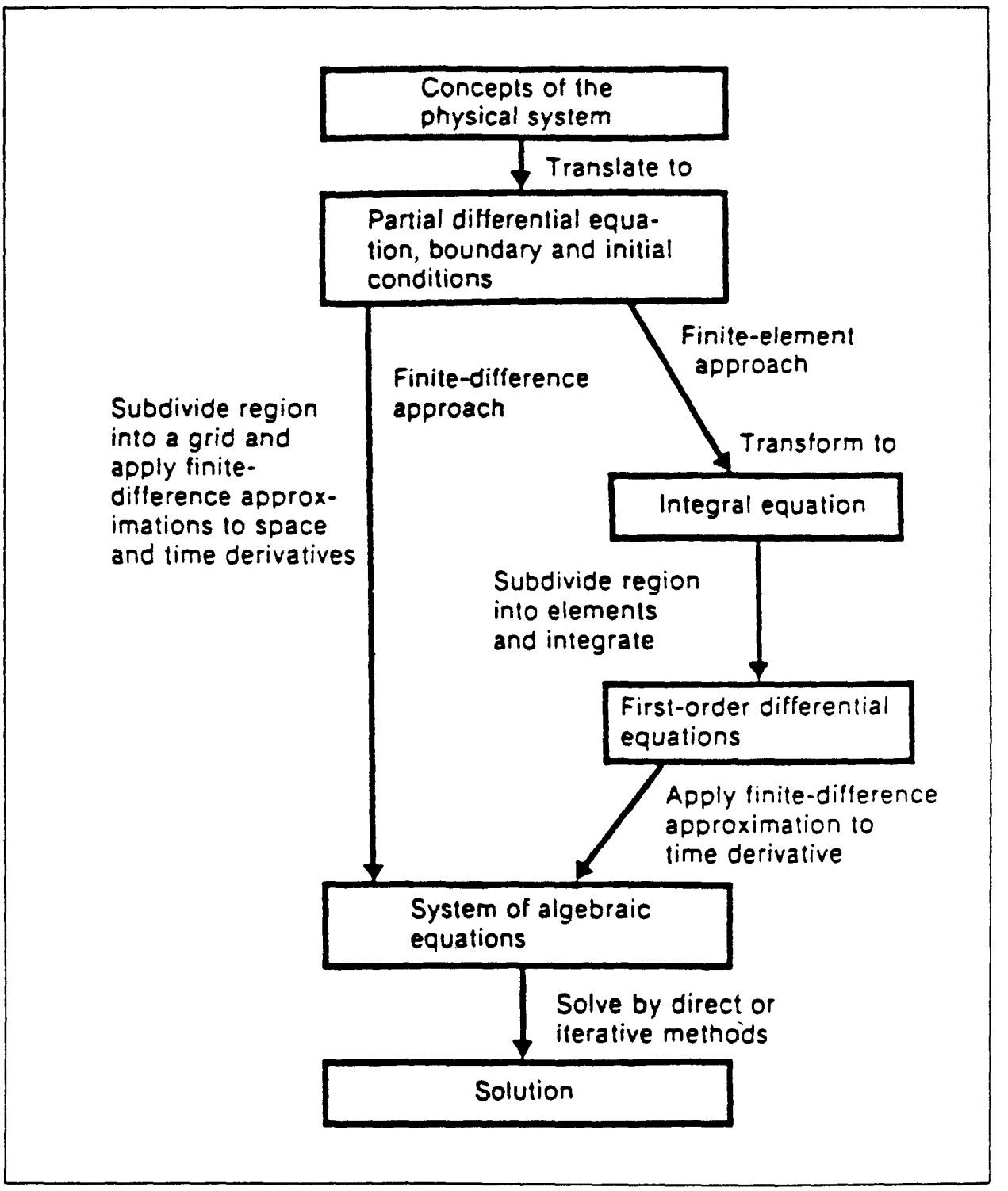


Fig. 14. Generalized model development by finite-difference and finite-element methods (after Mercer and Faust 1981).

FLOW MODELS

Groundwater flow models simulate the movement of one or more fluids in porous or fractured rock systems. One fluid is always water and the other may be an immiscible liquid such as a non-aqueous phase liquid (NAPL). Most existing groundwater models consider only the flow of water in saturated or variably saturated porous systems. Increasingly, research is concerned with multiphase flow of immiscible liquids and water and with flow and transport in fractured media.

The mathematical model for groundwater flow is derived by applying principles of mass conservation (resulting in the continuity equation) and conservation of momentum (resulting in the equation of motion; Bear 1972, 1979; Figure 15). The generally applicable equation of motion in groundwater flow is Darcy's linear law for laminar flow, which originated in the mid-nineteenth century as an empirical relationship. Later, a mechanistic approach related this equation to the basic laws of fluid dynamics (Bear 1972). An increasing number of models use a nonlinear equation of motion to describe flow around well bores in large fissures and in very low permeable rocks (non-darcian flow; Hannoura and Barends 1981, Huyakorn and Pinder 1983).

In order to solve the flow equation, both initial and boundary conditions are necessary (Franke et al. 1984). Initial conditions for saturated flow systems consist of given values for the piezometric head throughout the model domain. Initial conditions for variably saturated flow models are usually expressed in terms of pressure head. For most models, inclusion of initial conditions is only needed when transient simulations are performed. Boundary conditions for flow simulation may be any of three types: specified head (Dirichlet or first type), specified flux (Neumann type or second type), and head-dependent flux (Cauchy, mixed or third type) conditions. Boundary conditions are specified on the periphery of the modeled domain, either at the border of the modeled area or at locations within the system where system responses are fixed (e.g., connections with aquifer penetrating surface water bodies, or fluxes in/out of the system such as through wells).

Flow models have been developed for flow under both saturated and partially saturated conditions. Variably saturated models handle both conditions, using a single set of equations (the Richards' equation or a variant of it) (DeJong 1981, El-Kadi 1983). Models that have separate formulations for simulation of flow in the saturated zone and unsaturated zone are sometimes called coupled saturated-unsaturated zone models.

Complex liquid wastes often consist of multiple miscible and immiscible chemical components of varying density and viscosity. Saltwater intrusion is another density-driven flow phenomenon that impairs parts of many coastal aquifers and, increasingly, deep continental freshwater aquifers. Extensive evaluation of methods for analysis of saltwater intrusion is presented in Jousma et al. (1988). An overview of existing models for the latter type of use is given by van der Heijde and Beljin (1985).

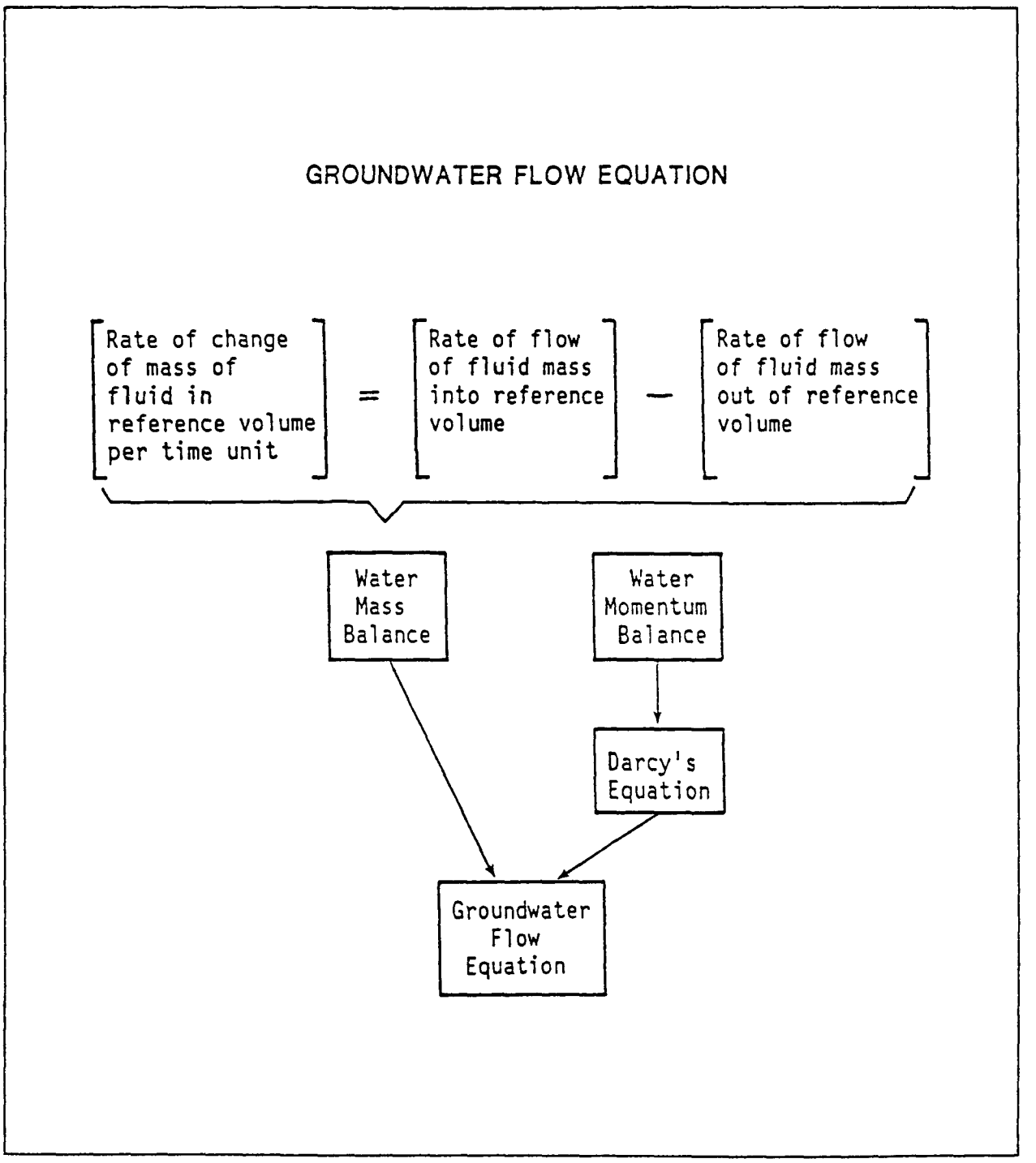


Fig. 15. Formulation of the groundwater flow equation.

IGWMC has compiled a comprehensive descriptive listing of models that address saturated, unsaturated, and multiphase flow. Appendix A covers saturated flow models; Appendix B covers models for unsaturated or variably saturated flow. The listings have been compiled from the Center's MARS model referral database, and have been limited to those models that are documented and readily available for third-party use.

Mathematical Formulation for Saturated Flow

The flow of a fluid through a saturated porous medium can be derived by combining the mass conservation principle with Darcy's law resulting in (Bear 1979):

$$S_s \frac{\partial h}{\partial t} - \nabla \cdot (K \cdot \nabla h) = 0 \qquad (1)$$

in which h is hydraulic head, K is hydraulic conductivity, and S_s denotes specific storage and is defined as

$$S_s = \rho g(\alpha + n\beta). \qquad (2)$$

Equation (1) is usually written as

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j}\right) - W^* = S_s \frac{\partial h}{\partial t} \qquad (3)$$

where W* denotes a source term expressed as a volume flow rate per unit volume with positive sign for outflow and negative for inflow. An overview of saturated flow models is presented in Appendix B.

Mathematical Formulation for Unsaturated Flow

Because air and water are immiscible fluids, when they coexist a discontinuity takes place between the two phases. The difference in pressure between the two fluids, called capillary pressure (P_c), is a measure of the tendency of the partially saturated medium to suck in water or to repel air. The negative value of the capillary pressure is called suction or tension. The capillary pressure head (ψ) is defined by (DeJong 1981)

$$\psi = \frac{P_c}{\rho g} \qquad (4)$$

The hydraulic head is given by

$$h = z - \psi \qquad (5)$$

in which z is elevation above an arbitrary datum.

The governing equation for unsaturated flow is derived by combining the mass balance principal with Darcy's law, ignoring compressibility of matrix, fluid, and air effects. The resulting equation, known as Richards' equation, is (DeJong 1981, El-Kadi 1983)

$$\nabla \cdot (K \nabla h) = F \frac{\partial h}{\partial t} . \qquad (6)$$

In equation (6), $K = K(\theta)$ is the hydraulic conductivity, θ is volumetric water content, h is total head, t is time, and F is moisture capacity defined as

$$F = \frac{d\theta}{dh} = - \frac{d\theta}{d\psi} \qquad (7)$$

The mathematical formulation and solution of the flow problem in the unsaturated zone require describing the hydraulic properties of soil, preferably in functional forms. The soil-water characteristic functions, $\psi(\theta)$ and $K(\theta)$, in which θ is the volumetric water content, is included in these properties. Hysteresis usually prevails in the relationship $\psi(\theta)$, i.e., a different wetting and drying curve (Figure 16). Soil air entrapment causes separation of the boundary drying and wetting curves at zero pressure. In fine-grained soils, subsidence or shrinking may cause the same effects. In general, simulation under hysteresis is difficult due to the existence of an infinite number of scanning, drying, and wetting curves, depending on the wetting-drying history of the soil. An example of the function $\theta(\psi)$ with no hysteresis is the form provided by van Genuchten (1978):

$$\theta = \theta_r + \frac{(\theta_s - \theta_r)}{[1 + |\alpha\psi|^N]^M} \qquad (8)$$

in which θ_s and θ_r are the saturated and residual water content, respectively, and α, N, and M are fitting parameters, with M related to N by

$$M = 1 - \frac{1}{N} . \qquad (9)$$

The hydraulic conductivity function $K(\theta)$ is represented by

$$K = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{1/2} \left\{1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{1/M}\right]^{M}\right\}^{2} . \qquad (10)$$

Other forms exist in the literature as well (see, e.g., El-Kadi [1985a,b]). Moisture capacity can be obtained by direct differentiation of equation (8). Another useful function, especially in the analysis of infiltration, is soil-water diffusivity, defined by

$$D_f = K / F \qquad (11)$$

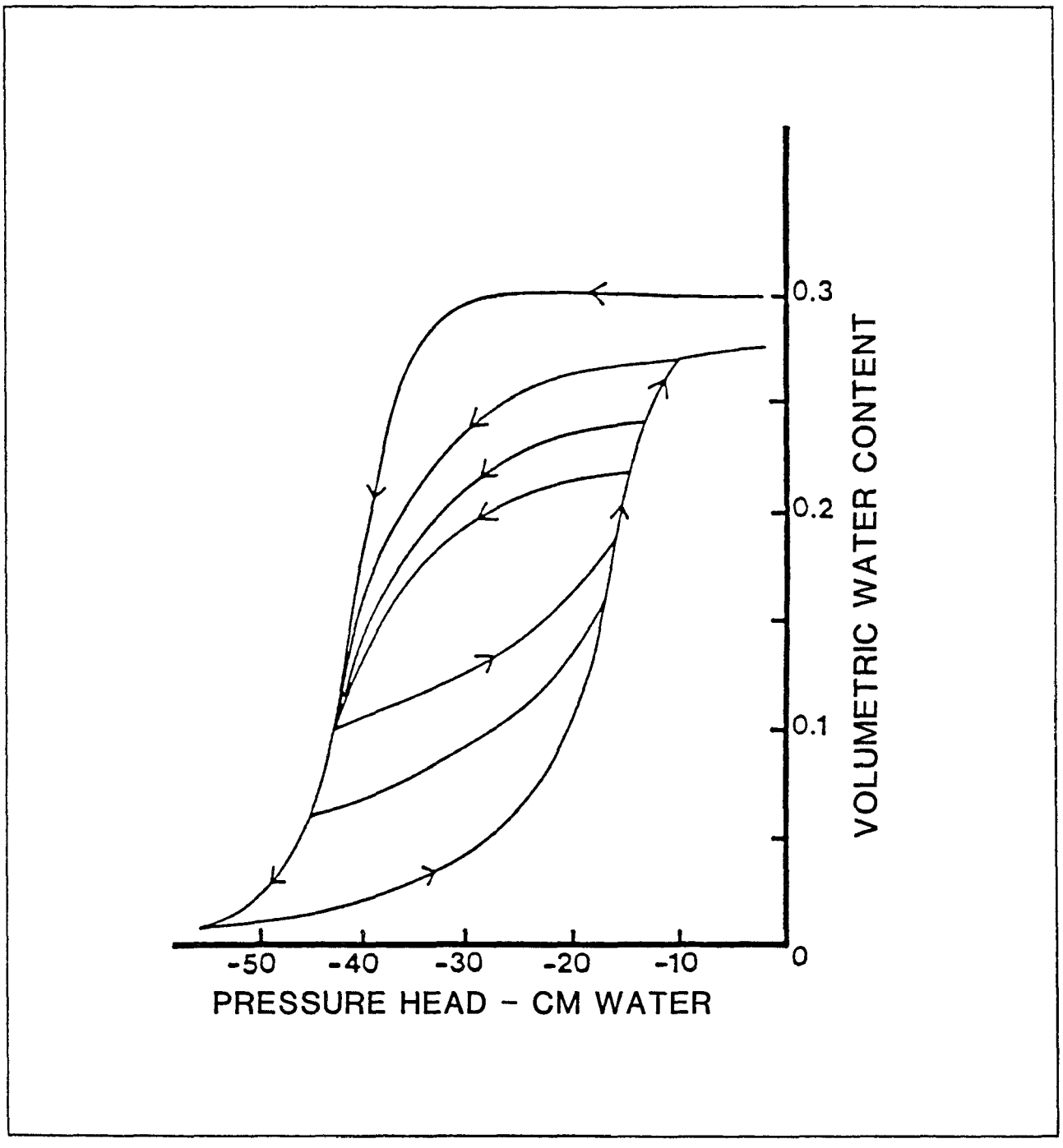


Fig. 16. Schematic relationships between water content and pressure head for various draining and wetting cycles (from El-Kadi and Beljin 1987).

which can be estimated explicitly from equations (7) and (10) (El-Kadi and Beljin 1987). An overview of variably saturated models is given in Appendix B.

Multiphase Flow

Fluids that migrate in the subsurface environment can be grouped with regard to their migration behavior as either miscible (mixes) with water or immiscible (does not mix) with water (Morel-Seytoux 1973, Parker et al. 1987). Miscible fluids form a single phase, while immiscible fluids form two or more fluid phases (a fluid is either a liquid or a gas). Such a grouping of fluids is essential for discussion purposes because the movement of two or more immiscible fluids is distinctly different from the simultaneous movement of miscible fluids. The flow of immiscible fluids gives rise to two-phase or multiphase flow and transport; miscible fluids give rise to single-phase flow and transport. The following discussion is based primarily on Kincaid and Mitchell (1986).

Migration patterns associated with immiscible fluids introduced at the soil surface (e.g., as a chemical spill) are schematically described by Schville (1984). The extent and character of migration depends on the chemical characteristics, the source volume, the area covered by the source, the infiltration rate, and the retention capacity of the porous medium. Retention capacity is a measure of the volume of immiscible liquid or nonaquous-phase liquid (NAPL) that can be held in the porous medium without appreciable movement. This volume is analogous to the volume of water prevented by the capillary force from draining because of the gravity force.

When the retention of the partially saturated soil column is not exceeded, the bulk of the liquid chemical contaminant will be retained in the soil column. Migration of the contaminant to the far-field environment will occur as a result of its dissolution in water; it may also move in a distinct vapor phase. Contaminated soil water arriving at the water table will be carried downgradient in the unconfined aquifer and in the capillary fringe. Figure 17 shows the ability of heterogeneous sediments within the partially saturated zone to laterally spread or broaden the contaminant plume with increasing depth. To estimate the retention capacity of the partially saturated soil column, the soil profile and moisture content must be known.

When the bulk volume of the chemical entering the soil exceeds the retention capacity of the partially saturated soil profile, the chemical will reach the water table in its liquid phase. Chemicals that are less dense than and immiscible in water, the so-called "floaters," will remain in the capillary fringe of the partially saturated zone and near the water table in the saturated zone, as indicated in Figure 18. Examples of this type of pollutant are gasoline and volatile organic solvents. Immediately beneath the spill chemicals can be forced below the water table and into the saturated zone by the pressure of the overlying liquid chemical mound (e.g., analogous to groundwater mound created by water disposal). As the plume migrates downgradient, the overlying pressure decreases and buoyant forces bring the lighter-than-air chemical up to the water table. The contamination will spread as a distinct liquid chemical phase and as a dissolved constituent in the groundwater. Contamination could also spread as a distinct chemical vapor phase. Certainly, some fraction of the chemical will be held in the porous medium by the reten-

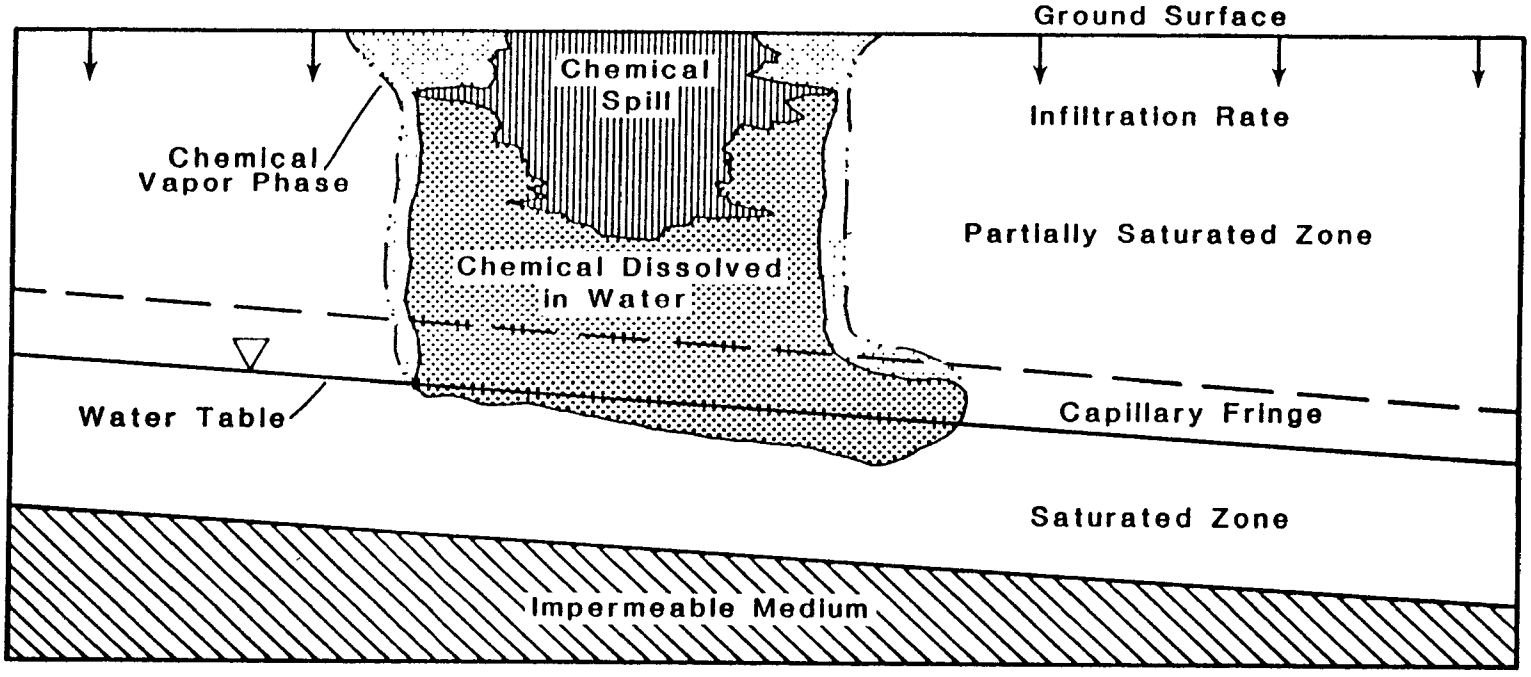


Fig. 17. Schematic diagram of a chemical spill of a volume less than the retention capacity of the partially saturated soil profile (from Schville 1984).

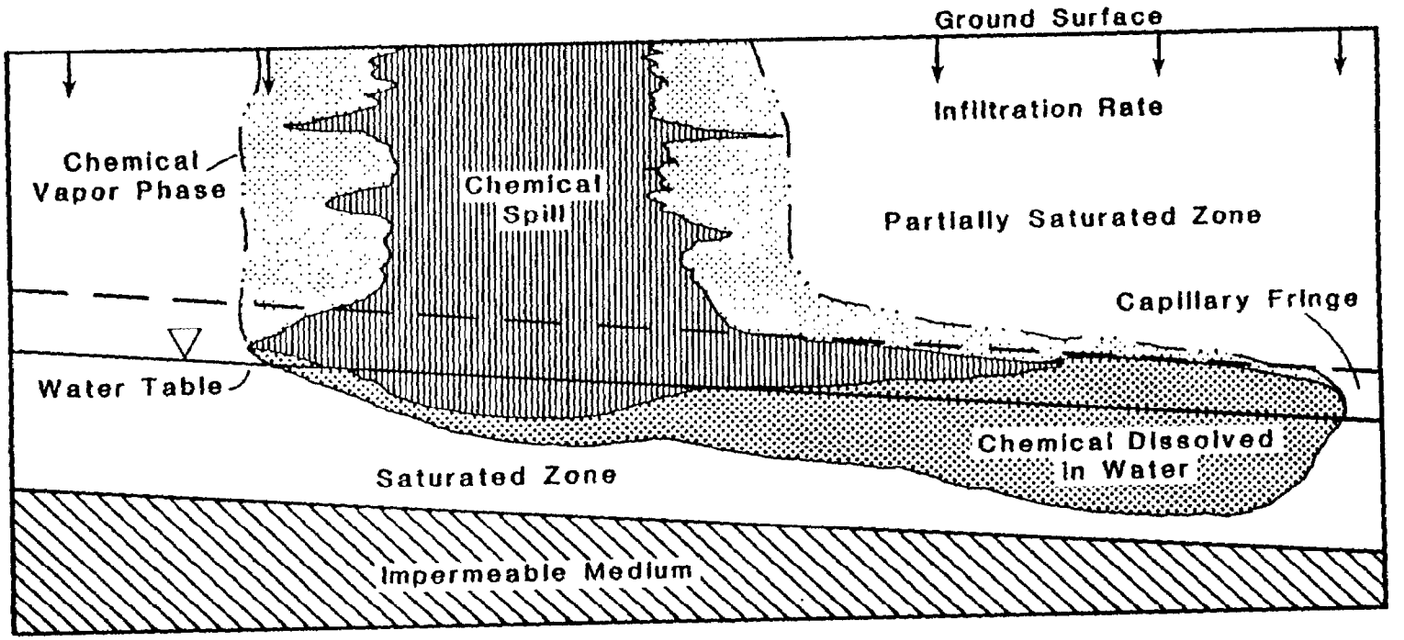


Fig. 18. Schematic diagram of a lighter-than-water chemical spill of a volume greater than the retention capacity of the soil (from Schville 1984).

tion capacity mechanism. Release of this fraction, as a dissolved constituent in soil water and groundwater, will be a long-term process.

As a substantial part of bulk volume of a heavier-than-water immiscible liquid (e.g., TCE) reaches the water table, the chemical will continue to move principally in the downward direction by displacing the groundwater. These liquids are called "sinkers." If the volume of the chemical moving into the saturated zone is greater than the retention capacity of the unconfined aquifer formation, the chemical will move through the entire saturated thickness of the unconfined aquifer. Depending on the physical/chemical properties of the chemical with respect to the impermeable formation, the chemical may continue its downward migration or form a mound above the impermeable bottom of the aquifer. Chemicals lying on the aquifer bottom will migrate by following the relief of the bedrock. These various aspects of the migration of the heavier-than-water chemical are shown in Figure 19.

As occurred in the partially saturated zone, heterogeneity within the saturated zone will cause the contaminant to spread laterally as the migrates vertically. Note that the slope of the bottom topography (i.e., relief of the bedrock) may not coincide with the groundwater gradient; the chemical is driven by its own gradient not the hydraulic gradient of the groundwater, and, hence, the chemical migration may actually move in a direction opposite to groundwater flow.

The existence of distinct fluid phases competing for the same pore space is governed by mass and momentum balance equations and data that uniquely specify the balance between the fluids in the soil environment. The wetting fluid is usually water; examples of a nonwetting fluid are mineral oil, chlorohydrocarbons, and soil air (Parker et al. 1987). Flow of each fluid is proportional to its potential gradient, the permeability of the medium, the fluid density and viscosity, and the portion of pore space (i.e., cross-sectional area) that the fluid occupies.

A fluid mass balance and Darcy's equation can be written for each of the fluids. When the detailed-flow phenomena in each fluid phase are of interest, as is the case with two liquids, the mass and momentum balance equations for each fluid should be solved. Consistent sets of saturation and potential for each fluid are obtained from such an analysis. However, when flow phenomena for only one of the two fluid phases are of interest, as is commonly the case with moisture movement in the partially saturated zone, the saturation and potential of the fluid of interest should be solved. The saturation of the second fluid can then be simply calculated given the porosity of the medium (i.e., given that it occupies the remaining pore space).

The relative permeability of the wetting and nonwetting fluids depends strongly on the degree of saturation (Dracos 1978, Parker et al. 1987). The curves describing the permeability of the fluids show the nonlinear behavior of fluids in a partially saturated environment. Unique curves exist for different fluids and media. In general, each fluid must reach a minimum saturation before it will flow. In the case of water and air, the minimum saturation for water is called the irreducible saturation. For moisture movement in the vadose zone, soil physicists have found that irreducible saturation is actually a function of the suction pressure applied and the length of time one is willing to wait for the soil column to respond. Thus,

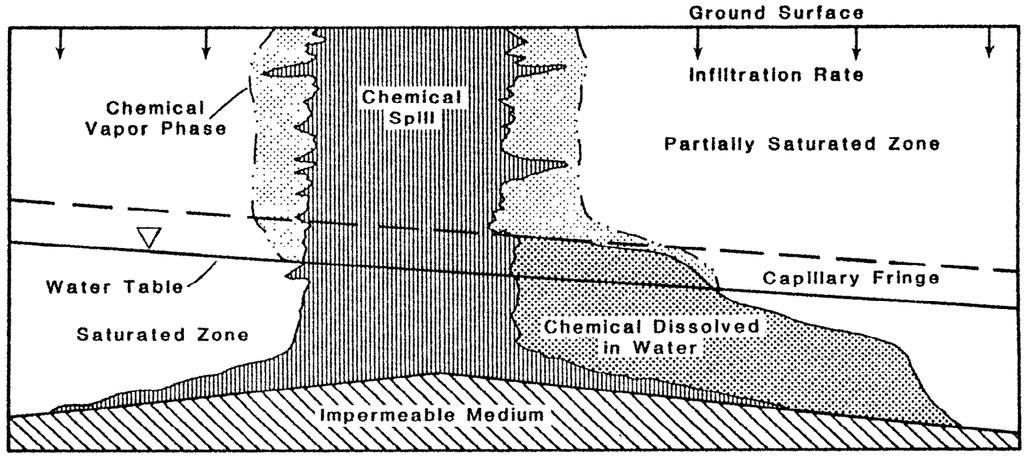


Fig. 19. Schematic diagram of a heavier-than-water chemical spill of a volume greater than the retention capacity of the soil (from Schville 1984).

irreducible saturation may not necessarily be single-valued. The wetting or nonwetting fluid must exceed its residual saturation before it will flow. Residual saturation is the measure of the ability of a soil to retain moisture and consequently the bulk of a chemical spill.

One of the more complex migration patterns that may occur involves three phases in the partially saturated zone (Kuppussamy et al. 1987). Water and chemical would exist as liquid phases and soil air would exist as a gaseous phase. The flow process is more complicated than the two-phase situation, although the same principles of mass and momentum balance apply. The individual fluids are immobile over relatively large areas of the saturation triangle, as shown in Figure 20; a relatively small central region exists over which all three phases are simultaneously mobile.

At low organic fluid saturations, a continuous organic phase may not exist and the organic fluid might be present as isolated globules surrounded by water. Such continuity is an essential assumption in virtually all existing models. In the current generation of models, discontinuity in a phase means that the relative permeability of the fluid goes to zero and that the model predicts no flow (Parker et al. 1987). In reality, however, migration of these isolated parcels of organic fluid can occur, resulting in a process termed "blob flow." This process is well known in tertiary oil recovery where the aim is to mobilize such "blobs," using injected surfactants and gases (e.g., Gardner and Ypma 1984). Existing mathematical models and codes cannot handle transport by way of globule migration.

Models and codes of organic chemical migration are commonly categorized as (1) those for which fluid physics of immiscible organic liquids are emphasized, and (2) those for which organics appear as miscible constituents in which chemical/microbiological reactions for dilute levels of contamination are emphasized. Existing models and codes can be used to model selected phases to the extent that vapor phase exchange and transport, geochemical reactions, and microbiological degradation can be incorporated in existing codes (i.e., insofar as the mathematical equations are unchanged by the addition of these processes and reactions). These models are based on the assumption that for each phase continuous flowpaths exist throughout the porous medium (Streile and Simmons 1986). A simplified version of such an approach is presented by Dracos (1978). The proposed model consists of vertical one-dimensional flow in the unsaturated zone through a column of radius R, under the source (Fig. 21) and a two-dimensional horizontal model for the low density liquid atop the watertable. For the miscible component in the plume a common 2D solute transport model is used, taking the source term from the 1D vertical column model. That it is not easy to make simplified modeling approaches work successfully for real-world phenomena is demonstrated by the Bartz and Käss experiment (Fig. 22) in which the bulk oil continues to advance slowly after 120 days, but the outmost boundary of detectable solutes is retreating, resulting in a 120-day contour being located outside the 360-day contour (Dracos 1978).

Petroleum industry models (Aziz and Settari 1979) do not appear to be readily applicable to organic transport analyses. These codes address only fluid flow phenomena and neglect entirely transport and attenuation phenomena. Petroleum industry codes may only be useful in regard to the theory and methods they embody for simulating multiphase, immiscible-fluid flow.

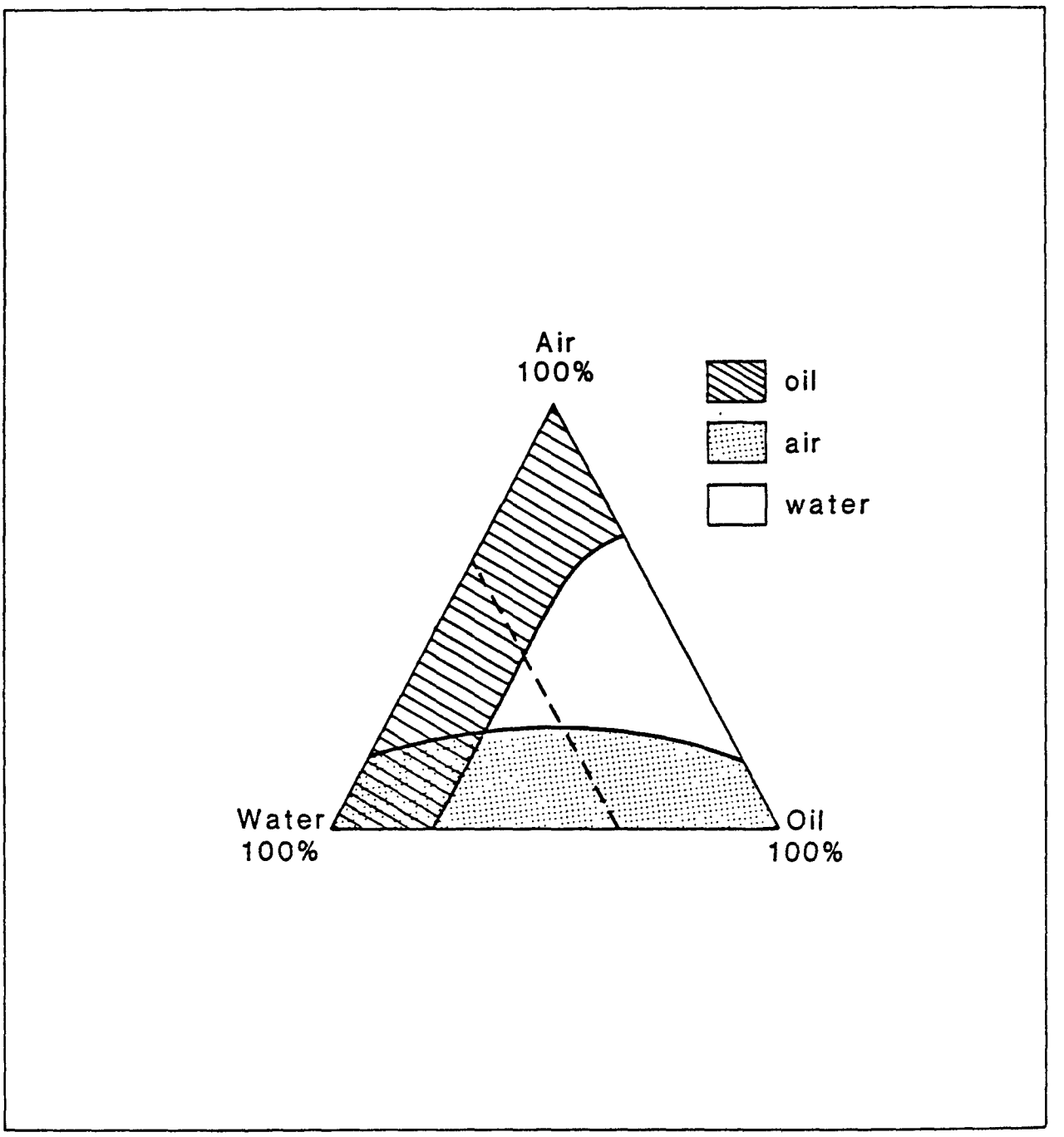


Fig. 20. Funicular zones for three immiscible fluids.

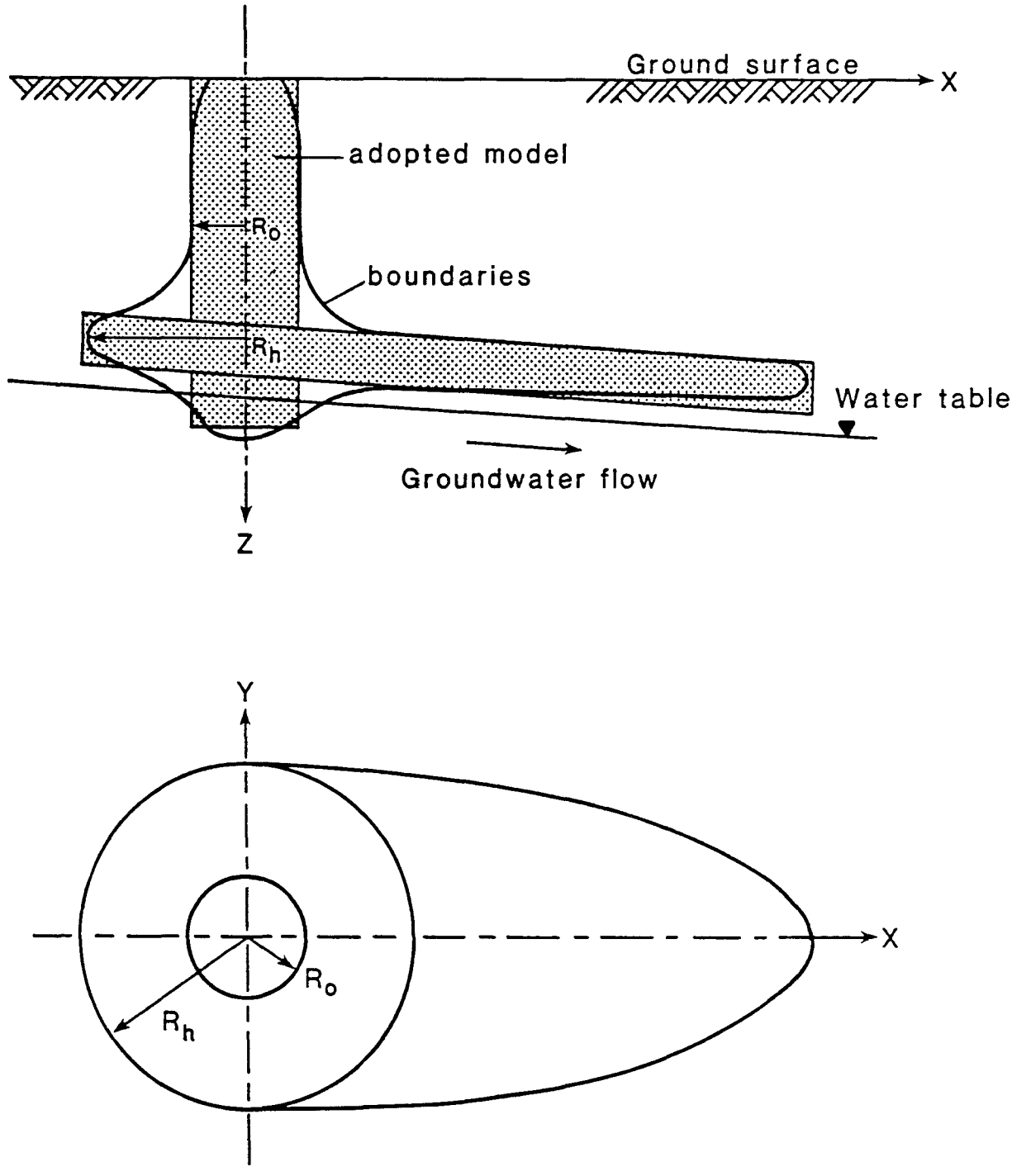


Fig. 21. Schematized vertical infiltration and horizontal spreading of the bulk of a low-density hydrocarbon atop the water table (after Dracos 1978).

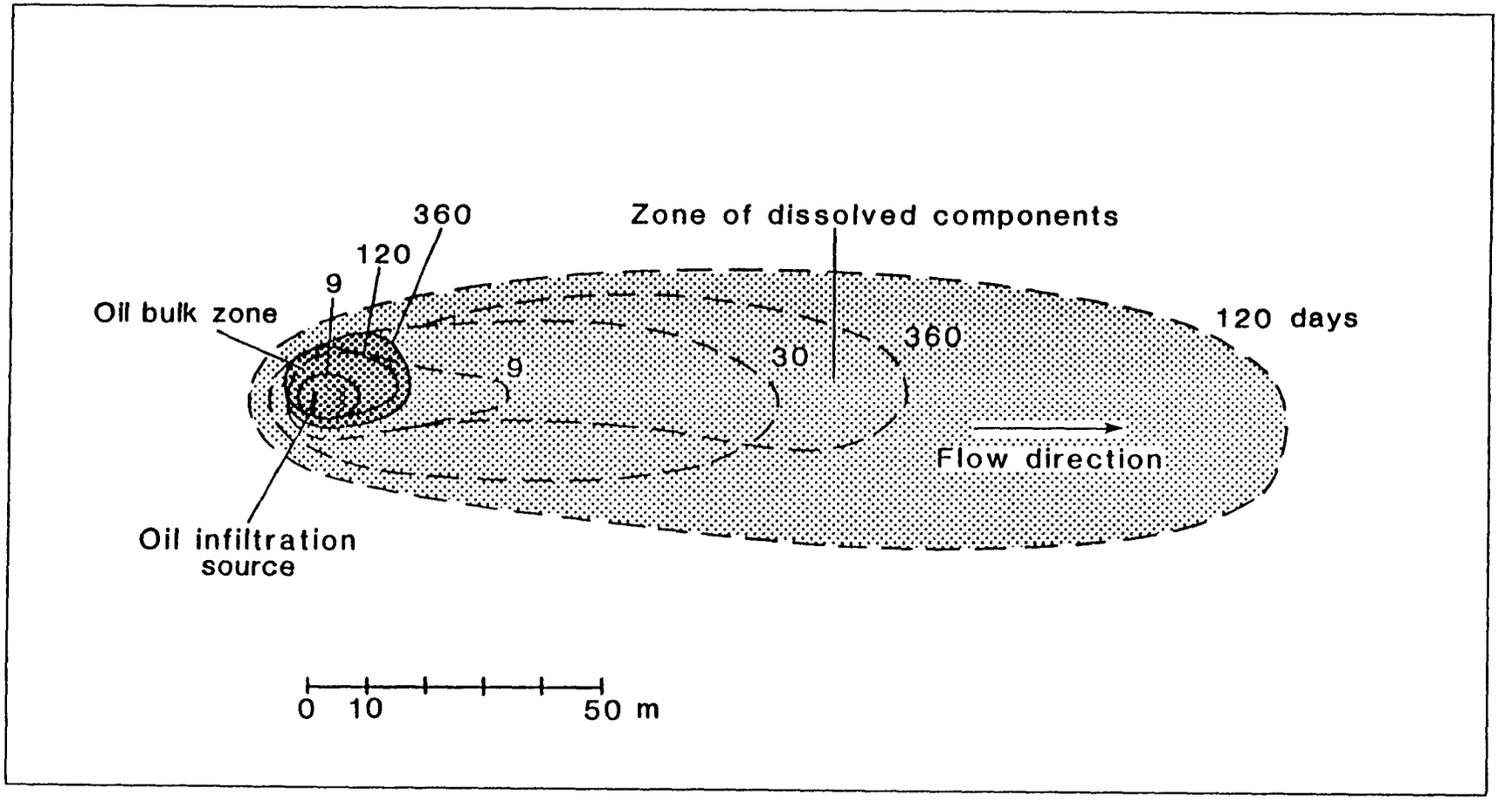


Fig. 22. Oil bulk zone and spreading of dissolved components in groundwater from a field experiment by Bartz and Käss (after Dracos 1978).

Experimental models for more complex systems, documented recently, include finite-element formulations by Abriola and Pinder (1985a, 1985b) and Kuppusamy et al. (1987) and a finite-difference formulation by Faust (1985). For further information on existing multiphase models, see Appendix G.

SOLUTE TRANSPORT MODELS

The groundwater transport of dissolved chemicals and biota such as bacteria and viruses is directly related to the flow of water in the subsurface. Many of the constituents occurring in groundwater can interact physically and chemically with solid phases such as clay particles, and with various dissolved chemicals. As a consequence, their displacement is both a function of mechanical transport processes such as advection and dispersion, and of physicochemical interactions such as adsorption/desorption, ion-exchange, dissolution/precipitation, reduction/oxidation, complexation, and radioactive decay. Biotransformations taking place during transport can alter the composition of the groundwater significantly (Ward et al. 1985).

In modeling the transport of dissolved chemicals, the principle of mass conservation is applied to each of the chemical constituents of interest (Figure 23). The resulting equations include physical and chemical interactions, as between the dissolved constituents and the solid subsurface matrix, and among the various solutes themselves (Reilly et al. 1987, Konikow and Grave 1984). These equations might include the effects of biotic processes (Molz et al. 1986, Borden and Bedient 1986, Srinivasan and Mercer 1988). To complete the mathematical formulation of a solute transport problem, equations are added describing groundwater flow and chemical interactions, as between the dissolved constituents and the solid subsurface matrix, and among the various solutes themselves. In some cases equations of state are added to describe the influence of temperature variations and the changing concentrations on the fluid flow through the effect of these variations on density and viscosity.

Under certain conditions such as low concentrations of contaminants and negligible difference in specific weight between contaminant and the resident water, changes in concentrations do not affect the flow pattern (homogeneous fluid). In such cases a mass transport model can be considered as containing two submodels, a flow submodel and a quality submodel. The flow model computes the piezometric heads. The quality submodel then uses the head data to generate velocities for advective displacement of the contaminant, allowing for additional spreading through dispersion and for transformations by chemical and microbial reactions. The final result is the computation of concentrations and solute mass balances. In cases of high contaminant concentrations in waste water or saline water, changes in concentrations affect the flow patterns through changes in density and viscosity, which in turn affects the movement and spreading of the contaminant and hence the concentrations (heterogeneous fluid). To solve such problems through modeling, simultaneous solution of flow and solute transport equations or iterative solution between the flow and quality submodels is required (Voss 1984, van der Heijde et al. 1985a, Kipp 1987). Mass transport models which handle only convective transport are called immiscible transport models, whereas miscible transport models handle both convective and dispersive processes. Models that consider both displacements and transformations of contaminants are called nonconservative. Conservative models only simulate convective and dispersive displacements.

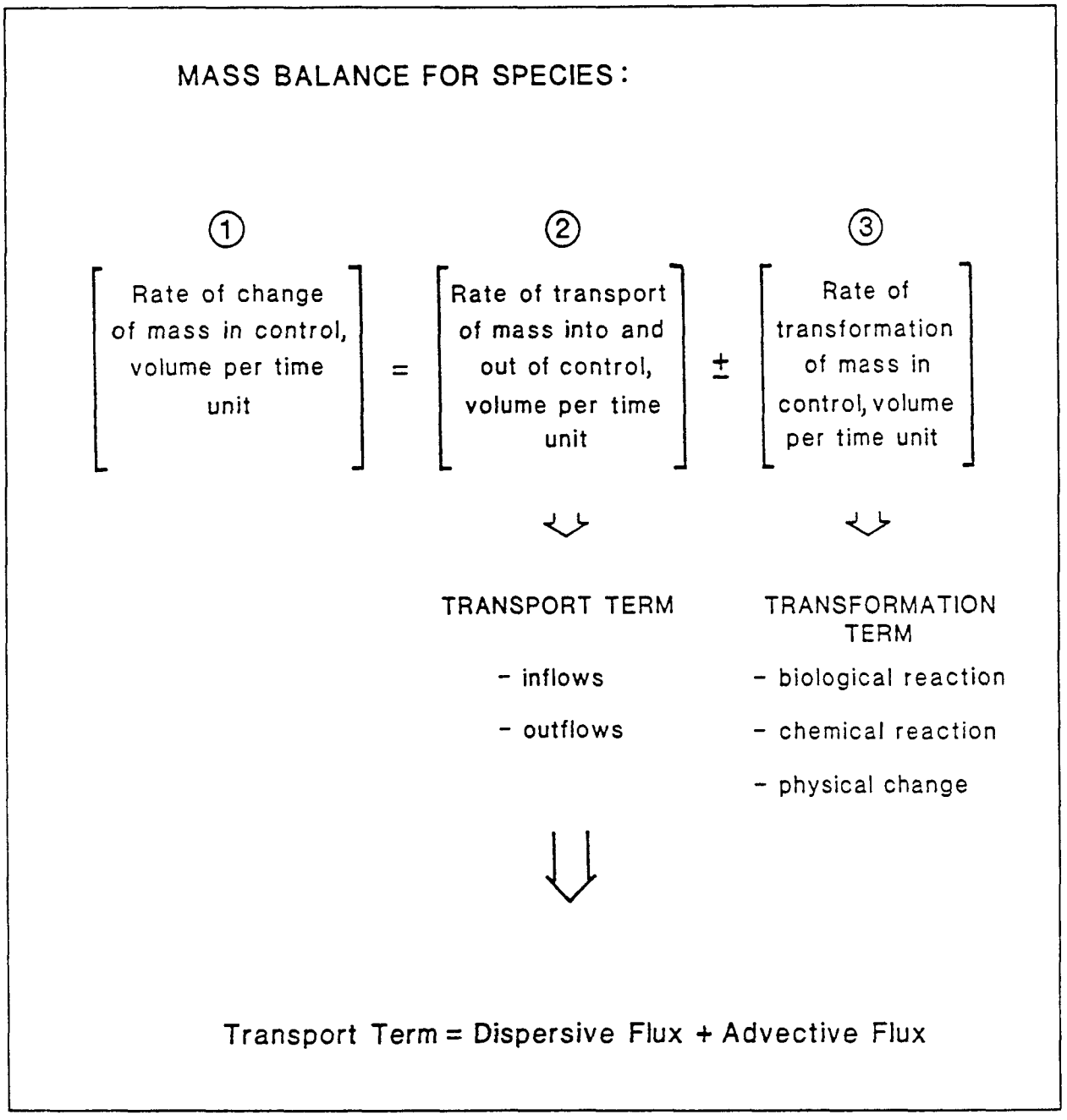


Fig. 23. Formulation of the solute transport equation.

There are two approaches for modeling multicomponent solutions. In the first approach, the interaction chemistry may be posed independently of the mass transport equations. The most widely used form of this approach is the coupling of the transport equation with an equilibrium phase exchange reaction such as the Langmuir or Freundlich isotherm (Jennings et al. 1982). An alternative approach is to insert all of the interaction chemistry directly into the transport equations (Jennings 1987).

In general, current solute transport models assume that the reaction rates are limited and thus depend on the residence time for the contaminant, or that the reactions proceed instantaneously to equilibrium. Recently, various researchers have become interested in a more rigid, kinetic approach to incorporate chemical reactions in transport models.

Several difficulties impair both the credibility and the efficient use of mass transport models. One such difficulty is "numerical dispersion" in which the actual physical dispersion mechanism of the contaminant transport cannot be distinguished from the front-smearing effects of the computational scheme (Huyakorn and Pinder 1983). For the finite-difference method, this problem can be reduced by using the central difference approximation. Another numerical problem occurs as spatial oscillations (overshoot and undershoot) near a concentration front, especially for advection-dominated transport, sometimes resulting in negative concentrations. Remedies for these problems are found in the reduction of grid increments or element size or by using upstream weighting for spatial derivatives. The use of weighted differences (combined upstream and central differences) or the selection of other methods (e.g., MOC, RW) avoids the occurrence of these numerical problems. A problem inherent to all numerical techniques, although of a different order of magnitude, is numerical inaccuracy. This problem can be mitigated by grid refinement or selection of an alternative method (Huyakorn and Pinder 1983). For the random walk method, higher accuracies can be obtained by increasing the number of particles in the system (Uffink 1983, Kinzelbach 1986).

Another problem is related to the general use of mass transport models in conjunction with flow models. Although a pollution problem is typically three-dimensional, vertical averaging is frequently used, resulting in the utilization of a two-dimensional, horizontal mass transport model that is generally connected with a hydraulic flow model. Such models tend to underestimate peak values and thus may fail to predict dangerous concentration levels and critical arrival times of pollutants in wells that become polluted by surface or near-surface sources.

Appendix C presents an overview of available solute transport models.

Advection-Dispersion Equation

Processes that control the migration of solute are advection, hydrodynamic dispersion, geochemical and biochemical reactions, and radioactive and biological decay.

In the case of a conservative solute, no reactions such as adsorption occur between the solute and the solid phase. The rate of transport is equal to the seepage velocity. If the transport of solute is due only to advection, a sharp interface will separate the flow domain that contains the solute and

the native groundwater. However, this interface does not remain sharp due to hydrodynamic dispersion, which causes solute spread over a greater volume of aquifer than would be predicted by an analysis of groundwater velocity. That means shorter traveling time for a pollutant from the source of the point of observation. In the case of an instantaneous release of pollutants and if dispersion is significant, advective transport relates to the movement of the center of mass of the spreading (dispersing) plume (Figure 24).

Convection--

Convection, sometimes refered to as advection, is the solute movement with the bulk flow of the fluid (water). Estimation of convection is based on determination of fluid flow characteristics, flow paths, and velocity. In most cases involving unsaturated flow conditions, numerical solutions of the flow equation are needed to accurately describe the flow field.

Dispersion--

The term hydrodynamic dispersion describes the spreading of a solute at the macroscopic (Darcy) level by the combined action of mechanical dispersion and molecular diffusion (Figure 24; Bear 1972, 1979). Mechanical dispersion is caused by the changes in the magnitude and direction of velocity across any pore cross-section at the microscopic level. Pores differ in size and shape, also causing variation in the maximum velocity within individual pores, in addition to velocity fluctuations in space with respect to the mean direction of flow. This results in a complex spatial distribution of the flow velocity. Molecular diffusion results from variation of solute concentration within the liquid phase. Solute moves by the gradient of concentration from regions of higher to lower concentration.

In practice, dispersion is considered to be caused by both microscopic and macroscopic effects (Dagan 1986). The difficulties in quantifying dispersion are encountered because studies of flow through porous media are conducted on a macroscopic scale. Darcy's law, for example, is a macroscopic equation.

In general, flux due to mechanical dispersion is estimated by analogy to Fick's law, i.e., flux is proportional to concentration gradient (Bear 1972, 1979). Combining the two effects results in the equation

$$Q_c = -D'\nabla C \qquad (12)$$

in which D' is called the effective diffusion-dispersion coefficient or the coefficient of hydrodynamic dispersion. D' is estimated as the sum of the coefficients of mechanical dispersion, D, and molecular diffusion, D_m. D is a tensor usually having longitudinal and transverse components. D_m is expressed generally as a function of the molecular diffusion coefficient of a chemical species in pure water and a tortuosity factor accounting for the nonuniformity of the pore system and the degree of saturation (Bresler and Sagan 1981, Gupta and Battacharya 1986), namely,

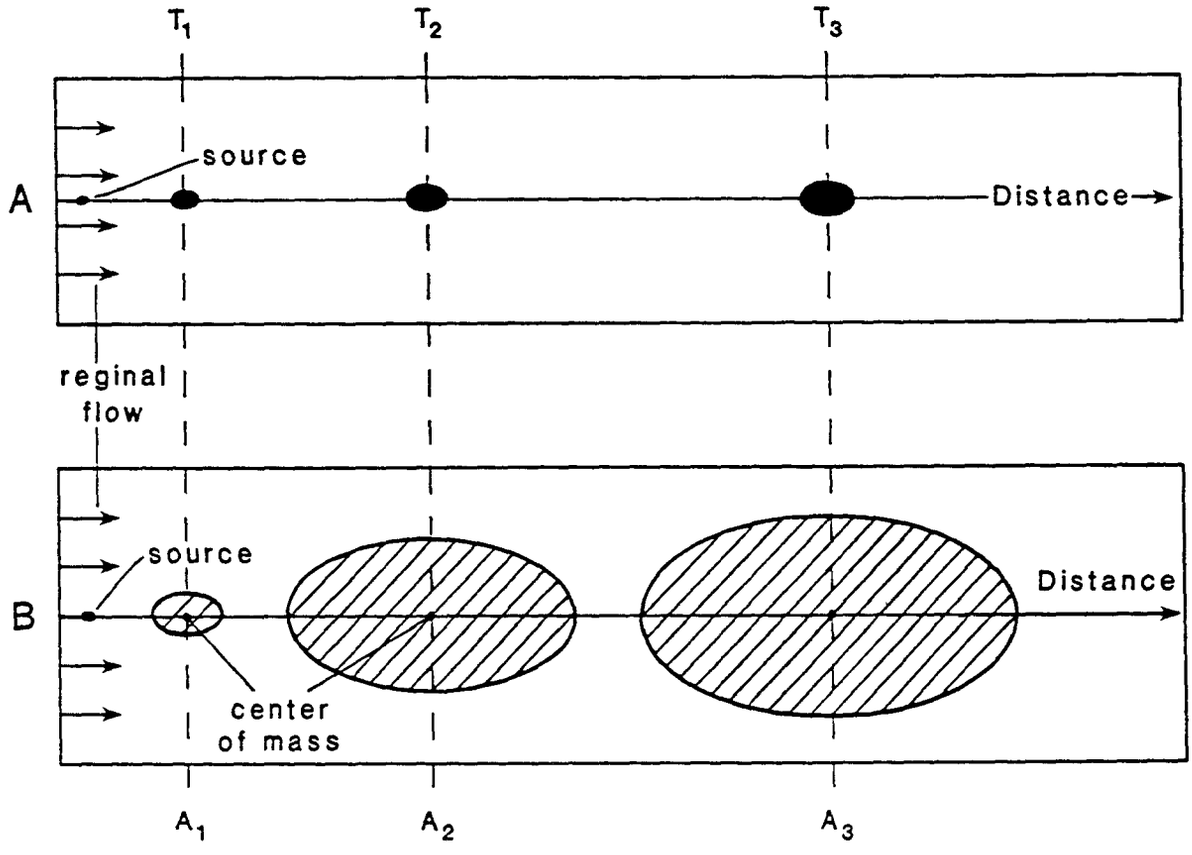


Fig. 24. Dispersion of a tracer slug in a uniform flow field at various times; the dispersion coefficients in case B are about 500 times greater than in case A (A, A_2, A_3 are traveled distances of center of mass of plume).

$$D_m = \eta_l(\theta) D_m' \tag{13}$$

in which η_l is the tortuosity factor and D_m' is the diffusion coefficient in pure water. One model for η_l is:

$$\eta_l = \frac{\theta^{10/3}}{n^2} \tag{14}$$

where n is porosity. Equation (14) is similar to that concerning air diffusion, as proposed by Millington and Quirk (1961).

Written in tensor form, the coefficient of hydrodynamic dispersion can be expressed as:

$$D'_{ij} = D_{ij} + D_m \delta_{ij} \tag{15}$$

where D_{ij} is the coefficient of mechanical dispersion, D_m is the coefficient of molecular diffusion, and δ_{ij} is the unit tensor.

The contribution of molecular diffusion to hydrodynamic dispersion is small when compared to mechanical dispersion and for any practical purpose may be neglected. The major ions in groundwater (Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, HCO_3^-, SO_4^{2-}) have diffusion coefficients in the range 1×10^{-9} to 10^{-9} m^2/s at 25°C (Robinson and Stokes 1965). However, its effects cannot be neglected for underground injection of hazardous wastes where the injection rates are in the order of centimeters per year for very fine soils (e.g., clays).

The coefficient of mechanical dispersion is usually expressed as a function of the velocity of groundwater and to the coefficient α_{ijkm}, called the dispersivity of the porous medium (Bear 1972, 1979). The dispersivity is a property of the geometry of the solid phase.

For isotropic porous media, the following equation can be derived (Bear 1979):

$$D_{ij} = \alpha_T \bar{V} \delta_{ij} + (\alpha_L - \alpha_T) \frac{\bar{V}_i \bar{V}_j}{\bar{V}} \tag{16}$$

where α_L and α_T are the longitudinal and lateral dispersivity, δ_{ij} is the Kronecker delta, $\bar{V}_i$ and $\bar{V}_j$ are components of the flow velocity in the i and j direction respectively, and $\bar{V} = |\bar{v}|$, the magnitude of the flow velocity or in Cartesian coordinates with velocity components $\bar{V}_x$ and $\bar{V}_y$

$$D_{xx} = \alpha_T \bar{V} + (\alpha_L - \alpha_T) \frac{\bar{V}_x^2}{\bar{V}} \tag{17a}$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{\bar{V}_x \bar{V}_y}{\bar{V}} \tag{17b}$$

$$D_{yy} = \alpha_T \bar{V} + (\alpha_L - \alpha_T) \frac{\bar{V}_y^2}{\bar{V}} \tag{17c}$$

$$D_{zz} = \alpha_T \bar{V}. \tag{17d}$$

If one of the axes coincides with the direction of the average uniform velocity $\bar{V}$, for example the x-axis, equations (17a-d) become

$$D_L = D_{xx} = \alpha_L \bar{V} \tag{18a}$$

$$D_T = D_{yy} = D_{zz} = \alpha_T \bar{V} \tag{18b}$$

where D_L and D_T are the coefficients of longitudinal and transversal dispersion, respectively.

Dispersivity is influenced by vertical and horizontal permeability, permeability variations, and degree of stratification (Güven et a. 1984, Black and Freyberg 1987). Because large solute plumes encounter more permeability variations than small plumes, dispersivity tends to increase and to approach some maximum asymptotic value (Gelhar et al. 1979). The difference between dispersivity values measured in the laboratory and evaluated in the field may be attributed to the effects of heterogeneity and anisotropy (Pickens and Grisak 1981a,b, Neuman et al. 1987). The values obtained from tracer tests are equivalent dispersivities that represent dispersion between the measuring point and the injection point (Anderson 1984).

Because of the difficulties in measuring dispersivity, both longitudinal and lateral dispersivities are often determined during calibration of the model. The common assumption is that the medium is isotropic with respect to dispersivity, which implies isotropy with respect to hydraulic conductivity. In practice, this is acceptable because most models used for solving field problems are two-dimensional with vertically averaged hydraulic properties and because generally the horizontal hydraulic conductivity is much larger than the vertical hydraulic conductivity. It should be noted that increasingly stochastic formulations are used to describe the dispersion process (Gelhar 1986, Smith and Schwartz 1980, Uffink 1983).

The partial differential equation for solute transport, including dispersion, convection, and a sink/source term may be expressed as (e.g., Anderson 1984)

$$\underset{\text{[dispersion]}}{\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_i}\right)} - \underset{\text{[convection]}}{\frac{\partial}{\partial x_i}\left(C\bar{v}_i\right)} - \underset{\text{[sink/source]}}{\frac{C'W^*}{n}} = \frac{\partial C}{\partial t} \qquad (19)$$

where C is concentration of solute, C' concentration of solute in the source or sink fluid, D_{ij} coefficient of dispersion, and $\bar{v}_i$ seepage or pore velocity.

The seepage velocity is calculated as

$$\bar{v}_i = -\frac{K_{ij}}{n}\frac{\partial h}{\partial x_j} = -\frac{q}{n} . \qquad (20)$$

The hydraulic head, h, is obtained by solving equation (9) and q by equation (2).

Adsorption--

Chemicals may partition between volatilized, adsorbed, and dissolved phases. An adsorbed chemical will migrate away from the source of pollution at a different rate than a nonsorbed chemical.

If equilibrium-controlled sorption is considered for adsorption/desorption between solid and liquid phase, equation (19) may be expressed as (Konikow and Grove 1984)

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_i}\right) - \frac{\partial}{\partial x_i}\left(C\bar{v}_i\right) - \frac{C'W^*}{n} = \frac{\partial}{\partial t}\left(C + \frac{\rho_b}{n}S\right) \qquad (21)$$

where ρ_b is the bulk density of the solid and S is the concentration of solute adsorbed on the solid surface.

The relationship between adsorbed concentration (S) and liquid concentration at equilibrium (C) is called the adsorption isotherm:

$$S = S(C) \ . \tag{22}$$

This relationship is obtained in laboratory experiments where the temperature is kept constant and the reactions are allowed to reach equilibrium. Several types of models for adsorption or ion exchange isotherms exist. Most frequently used isotherms are

Linear $$S = K_1 C + K_2 \tag{23}$$

Langmuir $$S = \frac{K_1 C}{1 + K_2 C} \tag{24}$$

Freundlich $$S = K_1 C^{K_2} \tag{25}$$

where K_1 and K_2 are empirically derived constants. All adsorption models represent reversible adsorption reactions. Generally two or more transport equations have to be solved for multi-ion transport problems.

The simplest isotherm is given as

$$S = K_d C \tag{26}$$

where K_d is the distribution coefficient:

$$K_d = \frac{\text{mass of solute on the solid phase per unit of solid phase}}{\text{concentration of solute in solution}} \ .$$

Distribution coefficients for reactive nonconservative solutes range from values near zero to 10^3 ml/g or greater (Mercer et al. 1982).

Incorporating equation (26) into equation (21), the advection-dispersion equation is given in the form

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(C\bar{v}_i\right) - \frac{C'W^*}{n} = R\frac{\partial C}{\partial t} \tag{27}$$

where R, the retardation coefficient is given by

$$R = 1 + \frac{\rho_b}{n} K_d. \tag{28}$$

As a result of sorption, solute transport is retarded with respect to transport by advection and dispersion alone. Sorption reduces the apparent migration velocity of the center of a plume or a solute front ($\bar{v}_s$) relative to the average groundwater flow velocity ($\bar{v}_{gw}$), or

$$R = \frac{\bar{v}_{gw}}{\bar{v}_s} \geq 1 \tag{29}$$

For K_d values that are orders of magnitude larger than 1, the solute is essentially immobile. Sorption capacity of geologic deposits is given in this order: gravel < sands < silts < clays ≤ organic material (Mercer et al. 1982). If no sorption occurs, the retardation factor is equal to 1.

It should be noted that a (small) portion of the solute will move significantly faster than the plume center due to the heterogeneity of the rock.

Transformation/Degradation--

Transformation and degradation processes determine the fate and persistance of chemicals in the environment. The key processes include biotransformation, chemical hydrolysis, and oxidation/reduction. The transformation and degradation processes are generally lumped as a reaction term in the solute transport equation. Reactions are usually represented by an effective rate coefficient which depends on a number of variables such as organic matter content, water content, and temperature. For simplification purposes, however, a first-order constant rate is usually employed in the analysis. For decay it is written as (Konikow and Grove 1984)

$$\frac{\partial C}{\partial t} = - \mu C \tag{30}$$

in which μ is the rate constant.

The solute (tracer) may undergo radioactive or biological decay

$$\frac{\partial C}{\partial t} = - \lambda C \tag{31}$$

where λ is the decay constant and can be calculated if the half-life of the tracer($t_{\frac{1}{2}}$) is known:

$$\lambda = \frac{\ell n 2}{t_{\frac{1}{2}}} . \tag{32}$$

Including decay and retardation and assuming decay rates are the same for sorbed and mobile species, equation (27) becomes

$$\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_i}\right) - \frac{\partial}{\partial x_i}\left(c\bar{v}_i\right) - \frac{C'W^*}{n} - \lambda RC = R\frac{\partial C}{\partial t} . \qquad (33)$$

Biodegradation--

Biodegradation in groundwater refers to chemical changes in solute or substrate due to microbial activity. Reactions can occur in the presence of oxygen (aerobic) or in its absence (anaerobic). Research related to biodegradation include the work of Troutman et al. (1984), Borden et al. (1984, 1986), Borden and Bedient (1987), and Barker and Patrick (1985). Modeling efforts include the work of Sykes et al. (1982), Borden et al. (1984), Borden and Bedient (1986), Bouwer and McCarty (1984), Molz et al. (1986), and Srinivasan and Mercer (1988).

Studies indicate that the number of electrons must be conserved in all biochemical reactions (Srinivasan and Mercer 1988). In such reactions, a reduced product (called electron acceptor) exists whenever a product has carbon atoms in a higher oxidized state due to the loss of electrons. For example, in aerobic reactions oxygen is the electron acceptor and is reduced to water. In anaerobic systems NO_3^- is the electron acceptor and is reduced to NO_2^-, N_2O, or N_2.

Modeling approaches can be divided roughly into two: (1) an approach that uses the biofilm concept to simulate the removal of organics by attached organisms (e.g., Molz et al. 1986), and (2) an approach that assumes that microbial population and growth kinetics have little effect on the contaminant distribution (Borden et al. 1984, Srinivasan and Mercer 1988). Both approaches apply Monod kinetics (see e.g., Lyman et al. 1982), or a modified form of them, to reduce the required number of equations.

Application of the first approach by Molz et al. (1986) has resulted in a set of five coupled nonlinear equations that need to be solved simultaneously to calculate the following:

Concentration of substrate
Concentration of oxygen
Substrate concentration within the colony
Oxygen concentration within the colony
Number of organism colonies per unit volume of aquifer

Three of the five equations are partial differential equations and two are algebraic equations. Microcolony kinetic parameters are needed for the analysis. The authors applied their approach to a one-dimensional problem for illustration purposes and performed a sensitivity analysis. They concluded that biodegradation can have a major effect on the contaminant transport when proper conditions for growth exist.

Application of the second approach by Borden and Bedient (1984) and Borden et al. (1986) has resulted in three partial differential equations describing contaminant concentration, oxygen concentration, and concentration of microbes in the solution. The authors solved the system of equations for one- and two-dimensional problems dealing with hydrocarbon contamination. They developed a code (BIOPLUME II) that is a modification of an existing two-dimensional solute transport model based on the method of characteristics (Konikow and Bredehoeft 1978).

Volatilization--

Volatilization is defined as the loss of a chemical in vapor from soil and plant surfaces. This process is controlled by the availability of vapor at the soil surface and the rate at which this vapor is carried to the atmosphere. In addition to the saturated vapor pressure of the chemical under consideration, a number of factors affect the actual volatilization rate from the soil surface, including soils and atmosphere characteristic, and management practices. Interaction among these components is also a controlling factor.

Generally, chemicals can partition into adsorbed, dissolved, and vapor phases. The vapor density is related to solution concentration under an equilibrium condition by a linear relationship of the form (Hern et al. 1986)

$$C_G = K_H C \ , \tag{34}$$

which is known as Henry's law, where K_H is Henry's constant. A similar relationship was described earlier regarding partitioning into adsorbed and dissolved chemicals.

Vapor movement from the soil to the atmosphere is usually modeled by applying Fick's Law of diffusion (Hern et al. 1986). Chemical movement in gaseous form through soil is described by an extension of the same law. The vapor flux is related to concentration gradient by

$$q_v = - \eta_2(a) D_G \nabla C_G \tag{35}$$

in which η_2 is a tortuosity factor and D_G is the dispersion coefficient in air. Millington and Quirk (1961) defined η_2 empirically, by

$$\eta_2 = \frac{a^{10/3}}{n^2} \tag{36}$$

in which a is air content and n is soil porosity. Equation (35) can be added to the general solute transport equation as a sink term.

Plant Processes--

Vegetation is an integral part of the terrestrial ecosystem. Chemicals applied to land surfaces may be intercepted by plant leaves where volatilization, photolysis, or biodegradation occur in addition to absorption by the plant itself. At a later time, the chemicals may be washed off to the soil by rain or irrigation water, where they contribute to solute transport in the soil. Plant roots also affect the transport phenomena by uptaking the chemicals into the plant where they can accumulate in different parts of the plant. Chemicals may move to the leaves where they are subject to transformation and degradation processes. The remaining chemicals may return to the soil following plant death or leaf fall.

Additional modeling difficulties result from the dynamic nature of plants, caused by changes in their condition from the time of planting until harvesting. Also, stem and root penetration can influence the transport phenomena by changing the hydraulic properties of soil.

Plant models have been introduced by plant and soil scientists (see Thornley 1976, Tillotson et al. 1980, Campbell 1985). Molz (1981) compiled a list of extraction functions used by various researchers to represent water uptake by plant roots. An exponential depth function adequately describes the extraction patterns for a number of crops under relatively stable conditions, such as a fully developed crop under high frequency irrigation (Feddes et al. 1974). However, a simple uniform function may be employed for chemical transport within a large soil depth.

HEAT TRANSPORT MODELS

Analysis of heat transport in soils and groundwater aquifers is an important area of research and has many practical applications. Heat transport affects other transport processes directly and indirectly, e.g., contaminant transport. Conversely, heat transport might be affected significantly by other physical and chemical processes. Overlooking such interactive effects may lead to unacceptable errors. Direct effects on pollutant transport are attributed to, for example, changes in the soil/groundwater flow field due to freezing/thawing on the chemical transformation rates due to temperature changes. The indirect effects are due to the fact that some parameters, e.g., hydraulic conductivity, are to a certain extent heat dependent.

Major research activities of heat transport processes in the past concerned high temperature geothermal systems with the best conditions for energy production. Accordingly, attention has been paid to models for simulation of complex systems such as water-steam-rock (e.g., Grant et al. 1982). Further applications of research relevant to heat transport in the subsurface include aquifer thermal energy storage (Mercer et al. 1982). There, warm waste water (e.g., from cooling systems) is injected into a confined aquifer during the warm season. During the cold season, warm water is recovered and utilized for heating purposes. The resulting cold water is reinjected far enough to prevent accelerating the cooling process of the warm water. An efficiency of heat recovery of up to 60% has been reported in the literature (Molz et al. 1978).

Another area of growing interest related to heat transport concerns modeling multiphase transport under freezing/thawing soil conditions. Difficulties in mathematical formulation, in solution approaches, and in parameter estimation are currently major hurdles toward the development of practical solutions to this complex problem.

Mathematical formulation of the general transport problem in the subsurface involves a coupled system of equations describing the flow of water, heat, and solutes. The equations are nonlinear in principal, because the parameters are a function of at least one dependent variable (temperature) interrelated by equation of state. In such a case, only numerical techniques might provide a solution. Numerical methods used in heat transport models were reviewed, e.g., in the report of Pinder (1979); in more general terms,

heat transport models were described in Bachmat et al. (1978) and van der Heijde et al. (1985a).

This section reviews briefly the theory of flow of water and solute in the subsurface under nonisothermal conditions. Details of the formulations may be found elsewhere (e.g., Lunardini 1981 and Farouki 1986). An up-to-date list of available models is provided in Appendix D.

The Heat Transport Equation

Groundwater may appear as ice, liquid or steam, interacting with an aquifer. The heat transport equation is derived by applying the energy balance principles concerning the transport, storage, and external sources/sinks of heat. Dependent variables in this equation may be temperature or enthalpy. In general, a state of thermodynamic equilibrium is assumed, i.e., the temperature in different constituents (solids and fluids) is equal within the representative elementary volume for which the equations are derived. The processes that contribute to heat transport include conduction, convection, dispersion, radiation, evaporation/condensation, and freezing/thawing. Heat conduction occurs in all soil constituents, i.e., solids, water in different phases, and air. In air and vapor, heat conduction is caused by collision between molecules that increases their mean kinetic energy as heat moves from warmer to cooler regions. In liquid water, the same process occurs in addition to energy transfer by breaking and forming of hydrogen bonds. In crystalline solids, e.g., quartz, increased atomic vibration at one end will cause the neighboring atoms in the lattice to follow suit. Heat flux due to conduction is given by

$$Q_{cd} = \lambda_o \nabla T \tag{37}$$

in which T is temperature and λ_o is the thermal conductivity of the porous medium (water plus solid), defined as the rate which heat energy flows across a unit area of the soil due to a unit heat gradient, where $\lambda_o/\rho C_o$ is assigned thermal diffusivity (e.g., W.B. Bird, 1960, p. 246) in a porous matrix.

Free or forced heat convection contributes to heat transfer. Free convection develops due to the existence of a temperature gradient resulting in density changes. On the other hand, forced convection is due to currents of fluids that move through pores of soils as a result of head gradients. For a fluid with velocity V_w the convective flux is given by

$$Q_{cn} = V_w \rho_w C_w T \tag{38}$$

in which ρ_w and C_w are density and specific heat of the fluid, respectively.

Dispersion, sometimes referred to as lateral mixing or turbulent diffusion, is caused by mixing in the pore system. Dispersive heat flux is given by

$$Q_D = \rho_w C_w \delta \nabla T \tag{39}$$

in which δ is the heat dispersion coefficient

$$\delta = \beta |V_w|, \tag{40}$$

where β is heat dispersivity analogous to solute dispersivity, although their magnitudes may differ in the same aquifer, based on field measurement in France (de Marsily 1986).

Radiation, usually an unimportant process in heat transport in soils, is the emission of heat from bodies that have temperatures above absolute zero. Heat energy is emitted in the form of electromagnetic waves and travels across a vacuum as well as gases, liquids, or solids. The flow of heat depends mainly on the temperature of the radiating body, namely,

$$Q_R = \sigma \varepsilon A T^4 \tag{41}$$

which is known as the Stefan-Boltzmann law. In equation (41), A is the surface area, σ is a constant, and ε the emissivity of the surface ($0 < \varepsilon < 1$).

Heat transport caused by evaporation/condensation is due to the fact that water evaporation absorbs considerable latent heat (586 ca/g at 20°C). Local vapor pressure increases, causing water vapor to diffuse through interconnected pores to regions of lower pressure, where vapor may condense, releasing its latent heat. Heat flux due to evaporation/condensation is given by

$$Q_s = K_1 \cdot k_v \frac{x_w^s - x_w}{x_w^s} \delta' \tag{42}$$

in which K_1 is the heat flux needed for evaporation/condensation, k' is a velocity coefficient, δ' is a control parameter that depends on the soil temperature, x_w is the value of the existing mole fraction of water in the soil-air, and x_w^s is the same value for air that is in equilibrium with the liquid water in the soil.

Phase change, in the form of freezing and thawing, is accompanied also by gain or loss of latent heat. Latent heat loss is necessary during ice formation. The apparent specific heat of freezing soil is given by

$$\bar{C} = C_s + C_w \theta_w + C_i(\theta_t - \theta_u) + L \frac{\partial \theta_u}{\partial T} \tag{43}$$

where C_s, C_w, and C_i are specific heat of solids, water, and ice, respectively, θ_t is the total moisture content, θ_u is the unfrozen moisture content, and L is latent heat of freezing water. The expression in equation (43) is based on the assumption that the specific heat of unfrozen water is the same as that for water under standard conditions (20°C, 0,1 MPa).

Ignoring air movement, the general heat transport equation can thus be derived by applying the mass balance principal to yield

$$\nabla.\{Q_{cd} + Q_D + Q_{cn}\} = \frac{\partial}{\partial t} \{\sum [\Theta_j \rho C_j T\} + S_h \qquad (44a)$$

or

$$\nabla.\{[\lambda_o + \rho_w C_w \delta] \nabla T + V_w \rho C_w T\} = \frac{\partial}{\partial t} \{\sum[\Theta_j \rho C_j T\} + S_h \qquad (44b)$$

in which S_h is a source/sink term that includes radiation, evaporation/condensation, or freezing/thawing effects. The subscript j in equation (44) refers to unfrozen water and ice (i.e., j=w for water and j=i for ice). Simplified versions of equation (44b) have been utilized in the analysis, especially in the absence of phase change processes. For example, for a fully saturated aquifer, if heat conduction and density changes are neglected, and if heat capacity was taken as constant, the equation becomes

$$C_w[\nabla\cdot(\delta\nabla T + V_w T)] = \alpha_h \frac{\partial T}{\partial t} + S_h \qquad (45)$$

in which α_h is the heat capacity of the aquifer.

HYDROCHEMICAL MODELS

Hydrochemical models are used to analyze system geochemistry independent of physical mass transport processes. The models can simulate chemical processes that regulate dissolved species concentrations, including mixing, adsorption, ion-exchange, redox reactions, complexation, and dissolution/precipitation reactions.

The focus of this section is on thermodynamic models for systems at chemical equilibrium (though EQ3NR/6 and PROTOCOL [listed in Appendix E] contain submodels that do not require equilibrium assumptions). Equilibrium is rigorously defined for closed systems only, i.e., systems that cannot exchange matter with their surroundings. Since all natural groundwater systems are open systems, the time-invariant condition describing the chemical state of the groundwater system is steady-state, not equilibrium (Rice 1986). Therefore, application of thermodynamic equilibrium models to groundwater systems must be done with care. Although chemical equilibrium in some groundwater environments may be assumed for time scales of tens of hundreds of years (Morgan 1967), certain processes may not approach equilibrium for much longer periods of time; additionally, some reactions may be near equilibrium, while others in the same system are not.

Although a system may not be at equilibrium, the thermodynamic models may be used to indicate how close or far a reaction is from equilibrium; therefore, although equilibrium models do not indicate the rate at which a reaction occurs, they do yield a description of the state towards which the system is tending (Rice 1986).

Equilibrium models can be valuable tools in predicting the behavior of complex geochemical systems. They do have limitations, however, and only by understanding the conceptual as well as the computational model can they be properly applied and interpreted. The following discussion deals with the theoretical derivation on which the thermodynamic equilibrium models are based, and limitations of those models; recent articles by Nordstrom et al. (1979), Jenne (1981), Kincaid et al. (1984), and Nordstrom, Kirk, and Ball (1984) review the actual models and computer codes. An overview of currently available computer codes is included as Appendix E1 and E2.

Gibbs Free Energy and Equilibrium Constants

In any system, a process is determined to be at equilibrium when the energy function used to describe it is at a minimum. For a closed system at constant temperature (T) and pressure (P), the energy associated with a geochemical process is described by the Gibbs free-energy function (Denbigh 1971, Lewis and Randall 1961, Moore 1972), which is defined as the total Gibbs free-energy of the products (final state) minus that of the reactants (initial state)

$$\Delta G = cG_C + dG_D - aG_A - bG_B \tag{46}$$

for the general chemical reaction

$$aA + bB \longleftrightarrow cC + dD \tag{47}$$

where upper case letters represent the species, and lower case letters the appropriate stochiometric coefficients.

The Gibbs molar free-energy for any individual species is related to the activity a_i of the species by the expression

$$G_i = G_i^0 + RT \ln a_i \tag{48}$$

where G_i^0 represents the free-energy of the species in a standard state condition, and R is the gas constant.

The expression for ΔG in equation (46) can be rewritten in terms of equation (48) as

$$\Delta G = \Delta G^{0} + RT \ln \frac{a_C^{c} a_D^{d}}{a_A^{a} a_B^{b}} . \tag{49}$$

At equilibrium, the ratio of activities raised to the power of the respective stoichiometric coefficients is equal to the equilibrium constant, K (law of mass action), and the change in total free-energy, ΔG, is zero; therefore

$$\Delta G_R^{0} = -RT \ln K . \tag{50}$$

Electrolytes and Activity Coefficients

Because equilibrium constants are defined in terms of activities, or effective solute concentrations, it is necessary to relate these quantities to experimentally measurable concentrations. The relationship (Moore 1972)

$$a_i = \gamma_i m_i , \tag{51}$$

where γ_i is the activity coefficient and m_i the concentration of a component i considered to be the solute, is based on a standard state that obeys Henry's Law. The solution becomes ideal ($\gamma_i = 1$) at low solute concentrations:

$$\lim_{m_i \to 0} \frac{a_i}{m_i} = 1 . \tag{52}$$

For the case of more than one solute in solution, all the solutes must simultaneously conform to the limit in equation (52).

If the expression for activity in equation (51) is substituted into equation (48), the result may be written

$$G_i = G_i^{o} + RT \ln m_i + RT \ln \gamma_i , \tag{53}$$

where the terms $G_i^0 + RT \ln m_i$ represent the free energy of component i in an ideal solution, i.e., one that follows Henry's Law over the entire range of concentrations. Thus the term involving the activity coefficient is a measure of the real solution's deviation from ideality.

It is possible to calculate single-ion activity coefficients from only electrostatic considerations. This was first done successfully with the Debye-Hückel theory, which manages to provide surprisingly good results despite several severe contradictions and physically incorrect assumptions (Bockris and Reddy 1970). Essentially, the Debye-Hückel theory ignores short-range interactions between ions of the same charge, and thus its predictions become poorer for more concentrated solutions in which ions with the same charge increasingly affect each other, and those with opposite charge form ion pairs through electrostatic attraction (Robinson and Stokes 1959).

Virtually all current computer models are based on the idea of ion pairing, which was developed independently by Bjerrum (1926) and Fuoss and Kraus (1933, Fuoss 1958). With the inclusion of these short-range ionic interactions, the modified Debye-Hückel equation for species i is

$$\log \gamma_i = - \frac{A_\gamma z_i^2 I^{\frac{1}{2}}}{1 + B_\gamma a_i I^{\frac{1}{2}}}, \tag{54}$$

in which A_γ and B_γ are the Debye-Hückel constants that depend on dielectric constant and temperature, z_i is the ionic charge, a_i an ion size parameter, and I the solution's ionic strength, defined by the expression

$$I = \tfrac{1}{2} \sum_i z_i^2 m_i. \tag{55}$$

In equation (54) the numerator accounts for long-range coulombic interactions, the denominator for short-range interactions that arise from treating the ions as hard, finite-sized spheres. As a correction for short-range ion-solvent interactions as well as short-range ion-ion interactions that are not accounted for by the hard-sphere model, a linear term is often added empirically to equation (54) or to some variation of it. The extended Debye-Hückel equation which incorporates the linear term, is given by

$$\log \gamma_i = \frac{A_\gamma z_i^2 I^{\frac{1}{2}}}{1 + I^{\frac{1}{2}}} + b_i I \tag{56}$$

where b_i is an ion-dependent empirical constant. The Davies equation (Davies 1967), a modified form of the extended Debye-Hückel equation, given by

$$\log \gamma_i = - \frac{A_\gamma z_i^2 I^{\frac{1}{2}}}{1 + I^{\frac{1}{2}}} - 0.2I \tag{57}$$

is frequently used to determine γ_i since it is supposedly applicable to solutions of ionic strength up to 0.5 M (Stumm et al. 1982); the Debye-Hückel equation is valid only up to about 0.1 M. Thus computer models that calculate activity coefficients by either (or both) of these equations are restricted to fairly dilute ground waters.

Oxidation-Reduction Reactions

Of all the reactions included in any of the computer models, only a small fraction consists of oxidation-reduction reactions. The model REDEQL-UMD (Harriss et al. 1984), for example, lists only twenty-two redox couples, and its authors caution that the kinetics of many oxidation-reduction reactions may be slow.

The emf or Nernst potential (E) for any reaction involving electron transfer can be determined from the expression (Moore 1972)

$$E = E^o = \frac{RT}{nF} \ln \frac{a_C^a \, a_D^d}{a_A^a \, a_B^b} , \qquad (58)$$

where n is the number of electrons transferred, F is the faraday, and the chemical notation refers to the general reaction in equation (47). The term E° is the standard emf of the redox reaction and can be calculated from the standard electrode potentials of the half reactions that sum to the overall reaction (Latimer 1952).

The fact that oxidation-reduction reactions can be characterized electrochemically in this manner has led to the idea that a groundwater system's "redox state" can be described in terms of a single parameter, either an overall Nernst potential, usually designated Eh (Freeze and Cherry 1979), or the negative logarithm of the electron activity designated pe (Truesdell 1968) in analogy with pH. The idea that a single parameter like pe or Eh can characterize an entire system is based on the assumption that all the oxidation-reduction reactions occurring in the system are at equilibrium. That this is not true has been stated explicitly (Morris and Stumm 1967, Jenne 1981, Wolery 1983), but suggestions that a particular redox couple may be used as an overall indicator of the redox state of the system continue (Liss et al. 1973, Cherry et al. 1979).

Lindberg and Runnells (1984) have quantitatively demonstrated the inaccuracy inherent in characterizing an entire ground-water system by a single redox parameter. The field-measured Eh value for each of approximately 600 water analyses was compared with the Nernst potential calculated from the data on ten different redox couples by means of the computer model WATEQFC (Runnels and Lindberg 1981). As these same authors (Lindberg and Runnels 1984) state: "The profound lack of agreement between the data points and the dashed line [which represents equilibrium points] shows that internal equilibrium is not achieved. Further, the computed Nernstian Eh values do not agree with each other. . . . If any measured Eh is used as input for equilibrium calculations, the burden rests with the investigator to demonstrate the reversibility of the system."

Because many of the important oxidation-reduction reactions are very slow and some are even irreversible, it is virtually impossible that any natural-water system can reach equilibrium with respect to all of its redox couples. Improvements in this area of computer modeling will require the inclusion of experimental data for each of the major redox couples in the water system under study.

Limitations of Hydrochemical Models

Each reaction in the set listed for a particular model must be characterized by an equilibrium constant. In any geological environment there is an extremely large number of possible reactions, and this is reflected by the databases of many of the models, some of which consist of several hundred reactions. These include not only reactions occurring solely in the aqueous phase, but also heterogeneous reactions between dissolved species and solid phases, such as precipitation/dissolution and ion exchange, as well as oxidation/reduction and degradation reactions that may be catalyzed by microorganisms in the soil.

At least three fundamental problems are associated with such tabulations of thermodynamic data. A particular species may simply be omitted from the database, so even though it is present in the physical system being modeled, it will obviously not appear in the final speciation results nor will its effect on the speciation of other elements. The program WATEQ3 (Ball et al. 1981), for example, is an extension of WATEQ2 (Ball et al. 1979) through the addition of several uranium species, but the expanded database does not include vanadium, which frequently occurs naturally with uranium, and thus the influence of minerals containing both elements cannot be taken into account.

Even when the database does contain particular minerals, thermochemical data for them may not be known with very great accuracy. This problem is frequently compounded by other uncertainties such as nonstoichiometry, solution-dependent composition with respect to replaceable cations, metastable forms, and variation in free energy and solubility with the degree of crystallinity (Stumm and Morgan 1981).

And third, the tabulated thermodynamic data is also usually not checked for internal consistency. Because the data for a particular reaction may come from more than one source, there is no guarantee that all calculations were made with consistent values of the necessary auxiliary quantities or that the data satisfies the appropriate thermodynamic relationships. In a study done by Kerrisk (1981), experimental solubilities of $CaCO_3$, $CaSO_4$, and $BaSO_4$ in 0-4 M NaCl solutions were compared to those calculated using four different computer models: WATEQF (Plummer et al. 1976), REDEQL.EPA (Ingle et al. 1978), GEOCHEM (Sposito and Mattigod 1980), and SENECA2, a modification of the earlier SENECA (Ma and Shipman 1972). Although the ionic strengths exceeded the limitations of the modified Debye-Hückel and Davies equations, the study indicated that results for the four models frequently differed even at low ionic concentrations. Calculations on $CaCO_3$ by GEOCHEM differed markedly from experimental observations even below 0.5 M; one possible explanation for this is the inclusion of an equilibrium constant of about 4 for the formation of the ion pair $CaCl^+$. This particular ion pair is omitted from the other three computer models, and in fact Garrels and Christ (1965) note that at ordinary temperatures chloride forms no significant ion pairs with any major cation of

natural waters. This clearly points to some of the dangers inherent in the ion-air method employed in equilibrium models, and indicates another potential problem associated with the thermodynamic databases selected for the different geochemical models.

Modeling Non-Dilute Solutions

A different approach to the problem of ionic interactions in solution is the specific-interaction model (Pitzer 1973), which has been applied to seawater (Whitfield 1975, Eugster et al. 1980) and hydrothermal brines (Weare 1981, Barta and Bradley 1985). It has been long assumed that the results from Debye-Hückel theory could be extended by the addition of power-series corrections (Weare et al. 1982):

$$\log \gamma_i = \log \gamma_i^{DH} + \sum_j B_{ij}(I)m_j + \sum_j \sum_k C_{ijk}m_j m_k, \qquad (59)$$

where γ_i^{DH} is the Debye-Hückel activity coefficient and $B_{ij}(I)$ and C_{ijk} are the second and third virial coefficients respectively (Lewis and Randall 1961), the latter of which is required only for solutions of ionic strength greater than 3 M. Pitzer (1973) has succeeded in modeling the second virial coefficient B_{ij} as a function of ionic strength and has also developed a Debye-Hückel term of the form

$$\log \gamma_i^{DH} = - \frac{A_\gamma z_i^2 I^{\frac{1}{2}}}{1 + bI^{\frac{1}{2}}} + \frac{2}{b} \ln(1 + bI^{\frac{1}{2}}), \qquad (60)$$

which fits experimental data better than the extended Debye-Hückel term given by equation (56).

Although the specific-interaction model is more complicated mathematically, it has the distinct advantage of not explicitly including ion pairs for ions that are only weakly associated, such as Ca^{2+} and Cl^-. Instead, the second virial coefficient accounts for these weak associations through its dependence on the ionic strength (Weare et al. 1982). Weare and his coworkers (Harvie and Weare 1980, Eugster et al. 1980, Harvie et al. 1982, Harvie et al. 1984), have begun applying this model to simple electrolyte systems. The most complicated thus far is one containing only 11 different ionic species, but the preliminary results appear to be a significant improvement over calculations based on ion pairing. There is still considerable work to be done before the specific-interaction model can be applied to groundwater in general, but it clearly has the advantage of being able to treat more concentrated solutions than ion-pair theory. Pitzer's equations have already been or are currently being incorporated into at least three geochemical models: EQ3NR (Wolery 1983), SOLMNEQ (Kharaka and Barnes 1973), and PHREEQE (Parkhurst et al. 1980).

STOCHASTIC MODELS

Uncertainty due to the lack of information about the system or to the variable nature in space and time of certain properties or processes is increasingly incorporated in the analysis of groundwater systems. Incorporating information uncertainty in stochastic analysis can produce a best estimate of output (the mean) and a measure of the uncertainty of the estimate (the variance). On the other hand, if intrinsic uncertainty is included, the model results can describe head (for example) as a stochastic process resulting from an input (e.g., hydraulic conductivity) represented by a stochastic process. In other words, head is represented, as is the case with hydraulic conductivity, as a mean trend with superimposed fluctuations described by the covariance structure. In addition, questions regarding spatial structure, statistical homogeneity, and ergodicity of the system (see, e.g., Bakr et al. 1978) need to be addressed if intrinsic uncertainty is incorporated.

Recent review of the stochastic approach to analyze uncertainty due to intrinsic heterogeneity was introduced by Neuman (1982), El-Kadi (1984) and Freeze et al. (1989). Deterministic models fail because correct parameter values needed for models are not known at all locations other than those few available measurements. Recent research in stochastic analysis can be divided into: (1) a geostatistical approach to estimate uncertainty in input parameters (e.g., Hoeksema and Kitanidis 1985), and (2) a simulation approach to assess the impact of uncertainty of these parameters on model results (e.g., Bakr et al. 1978). In addition, the stochastic analysis has been used to study the physics of flow and transport in fractured and porous media. For example, it can be used to illustrate how heterogeneities affect flow patterns (Smith et al. 1989), to analyze the impact of spatial variability on macroscopic dispersion (e.g., Gelhar and Axness 1983, Smith and Schwartz 1984), and to estimate effective parameters that allow the representation of the true heterogeneous media by an equivalent homogeneous one (e.g., El-Kadi and Brutsaert 1985).

Two issues stand central in the stochastic approach.

The first issue is describing the spatial variability in probablistic terms. In general, statistical distributions of model parameters can be estimated through the use of the geostatistical approach to analyze available data (e.g., Hoeksema and Kitanidis 1985). Given a set of data points located at random in space, the geostatistical approach (also known as kriging) offers a best linear unbiased estimation of a regionalized variable (e.g., hydraulic conductivity) at various locations. A spatial structure is used in the analysis, through the variogram which indicates the degree of correlation between values of the variable as a function of distance. In general, an assumed distribution of the variable (e.g., normal or log-normal) is employed and the first few moments of that distribution are used as input to the stochastic simulation model. These moments include the expected value and the variance and covariance of the variable.

The second issue involves mathematical techniques to solve the stochastic equation. The available approaches can be divided into analytical, quasi-analytical, and numerical. The analytical techniques include derived distributions (Benjamin and Cornell 1970) that provide an explicit expression of the

probability distribution function (PDF) of the output variable (e.g., hydraulic head) as a function of the PDF for the input variable (e.g., hydraulic conductivity). This approach also includes the spectral analysis technique (Bakr et al. 1978, Gelhar and Axness 1983) that estimates the expected value and covariance of output parameters.

The quasi-analytical techniques include finite-order (first- or second-order) or perturbation analyses (Sagar 1978, Dettinger and Wilson 1981). They also provide expressions for the first few moments within a finite-element or a finite-difference framework. The numerical approach employs the Monte-Carlo technique, i.e., the repetitive solution of the deterministic problem for a large number of realizations, each with a set of parameters that is an equally probable representation of the actual set of parameters. The final product is a set of answers that can be analyzed to estimate the PDF or the first few moments of the distribution of the output variable. Example applications of the technique are presented by Smith and Freeze (1979) and El-Kadi and Brutsaert (1985).

Rather than a single answer that results from a deterministic model, the stochastic model provides a range of answers that can be expressed through a PDF or a number of the distribution moments.

A decision-theory framework based on the probabilistic structure of the measured variables can be used to assess the worth of data (Massman and Freeze 1987). An objective function that includes benefits, costs, and risks is optimized, allowing for assessment of the economic consequences of either planning alternative measurement strategies for a new site, or adding new measurements to an existing data collection strategy. When additional costs are no longer balanced by the risk reduction, additional measurements are not justified. This probabilistic modeling framework can also be used to make decisions regarding alternative actions, such as selecting between alternative sites for waste disposal or between alternative engineering designs for a specific site.

FLOW AND TRANSPORT IN FRACTURED ROCK

Fracture Systems

Metamorphic and igneous rock generally have very low matrix porosities. As a result, primary permeabilities are so small that they are often regarded as zero. Significant porosities and permeabilities, however, are developed through fracturing and weathering of the rock, especially in association with faults (Davis and DeWiest 1966). This type of permeability is referred to as secondary permeability. The average porosity of metamorphic rocks decreases rapidly with depth. Joints, faults and other fractures tend to close at depth because of the weight of the overlying material. However, some openings exist at all depths.

Sedimentary rock is often quite porous. Most fine-grained detrital rocks like shale, claystone, and siltstone have relatively high matrix porosities, but very low permeabilities (Davis and DeWiest). Coarser-grained sedimentary rock like sandstone can pair relatively high matrix porosity with a significant matrix permeability. Hydraulic properties of both types of sedimentary

rock might be enhanced largely if fractures are present. Furthermore, even in packed noncemented granular media, major cracks, macropores, and holes may be present. Such fractures occur over many length scales from microscopic to regional scale and have a multitude of geometrical characteristics.

As the original porosity and permeability of carbonate rock (mostly limestone and dolomite) are often modified (and reduced) rapidly after deposition, a wide range of matrix properties might be encountered in the field. Although original pore space might be retained in older deposits, other forms of porosity are more important such as fractures and solution openings created by dissolution of the carbonate rock along bedding planes.

Flow in Fractures

The flow behavior of fractured rocks is often characterized in some complex manner by the presence of discontinuities in the rock. These discontinuities can consist of cracks, fissures, fractures, joints, and shear zones and occur usually in sets of families with similar geometries (Witherspoon et al. 1987). Flow in such systems may take place through a channel network of interconnected fractures. (Streile and Simmons 1986). Flow may also occur simultaneously through the porous component of the media, if present. In the latter case, the flow system is often referred to as a dual porosity system with matrix porosity as primary porosity and fracture porosity as secondary porosity (Figure 25).

The major issues in analyzing fluid flow through a network of fractures where the rock matrix is essentially impermeable, are determining the permeability of the fracture system and establishing whether or not such networks behave more or less as a porous medium. It is often observed in the field that rock masses contain sets of discontinuous fractures of finite size within a single plane. As a result, the degree of interconnection between the assemblage of discontinuous fracture planes has a major influence on the hydraulic conductivity of the total system (Witherspoon et al. 1987). The density, or number of fractures per unit volume of rock, is another important feature. Finally, the orientation will determine those directions along which the fluids may flow within the rock mass. Thus, characterization of a fracture system is considered complete when each fracture can be described in terms of its size, location, effective aperture and orientation (Figure 26) and the global geometry of the system in terms of interconnectivity of fractures is established. It should be noted that the extent of aquifers is commonly one to three orders of magnitude larger than the aquifer thickness; fractures may extend over the vertical thickness of the aquifer, but rarely traverse its length.

To understand fluid flow in rocks of low permeability, it is necessary to investigate directional characteristics of hydraulic properties. In many of these hydrogeologic systems, the major channels of mass transport are fractures. Fracture systems can be grouped into continuous and discontinuous systems. Continuous systems consist solely of conductive fractures that are very long compared to the region under study. Discontinuous systems consist of finite-length fractures. The pore region of discontinuous systems consists of dead-end zones, isolated zones and conductive zones. Part of the pore region in continuous systems may become nonconductive due to the orientation of the hydraulic gradient (Endo and Witherspoon 1985) (Figure 27) or local flow direction might be altered significantly (Figure 28).

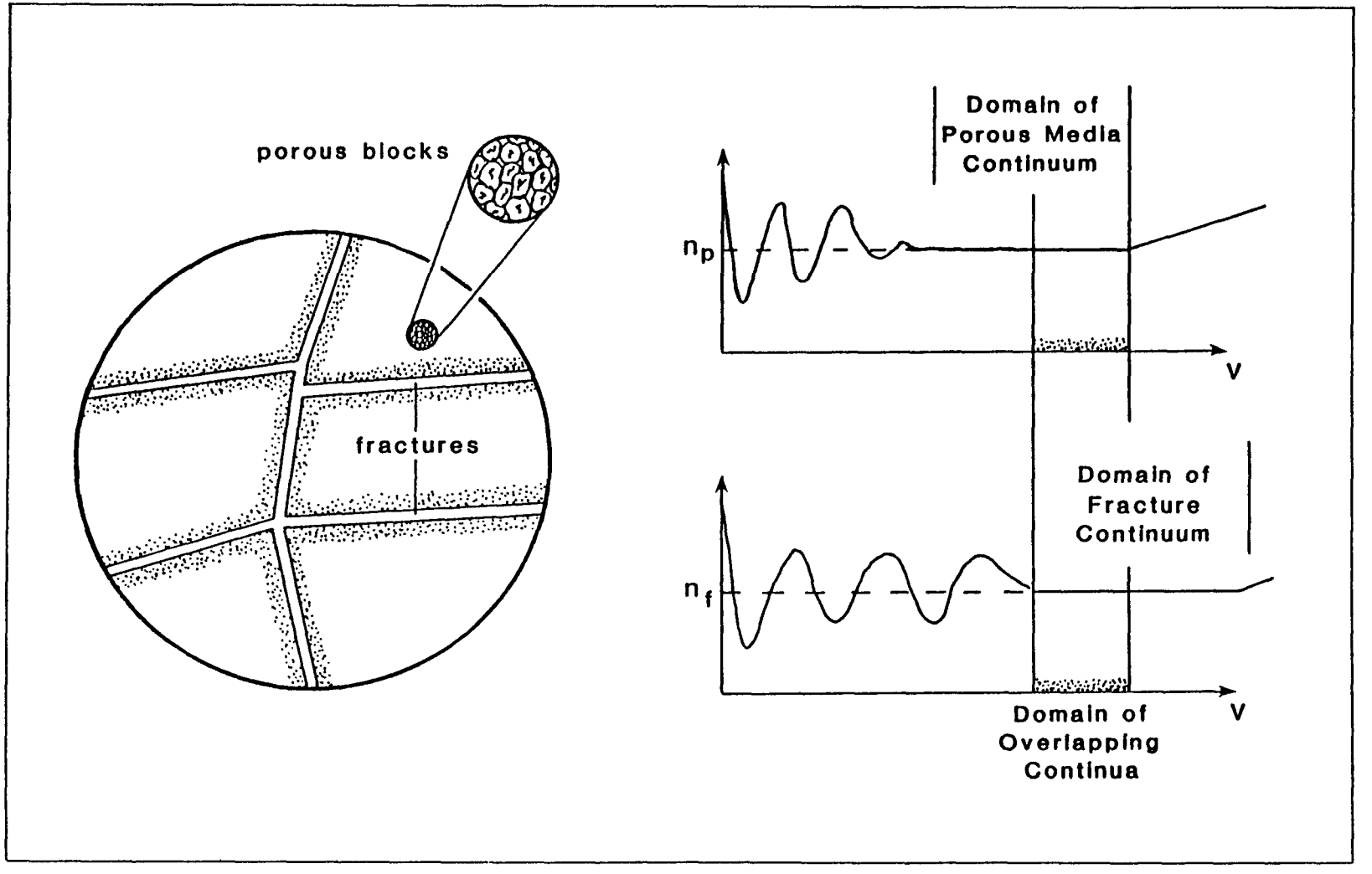


Fig. 25. Dual porosity and scale where continuum approach applies (after Huyakorn 1987, pers. comm.).

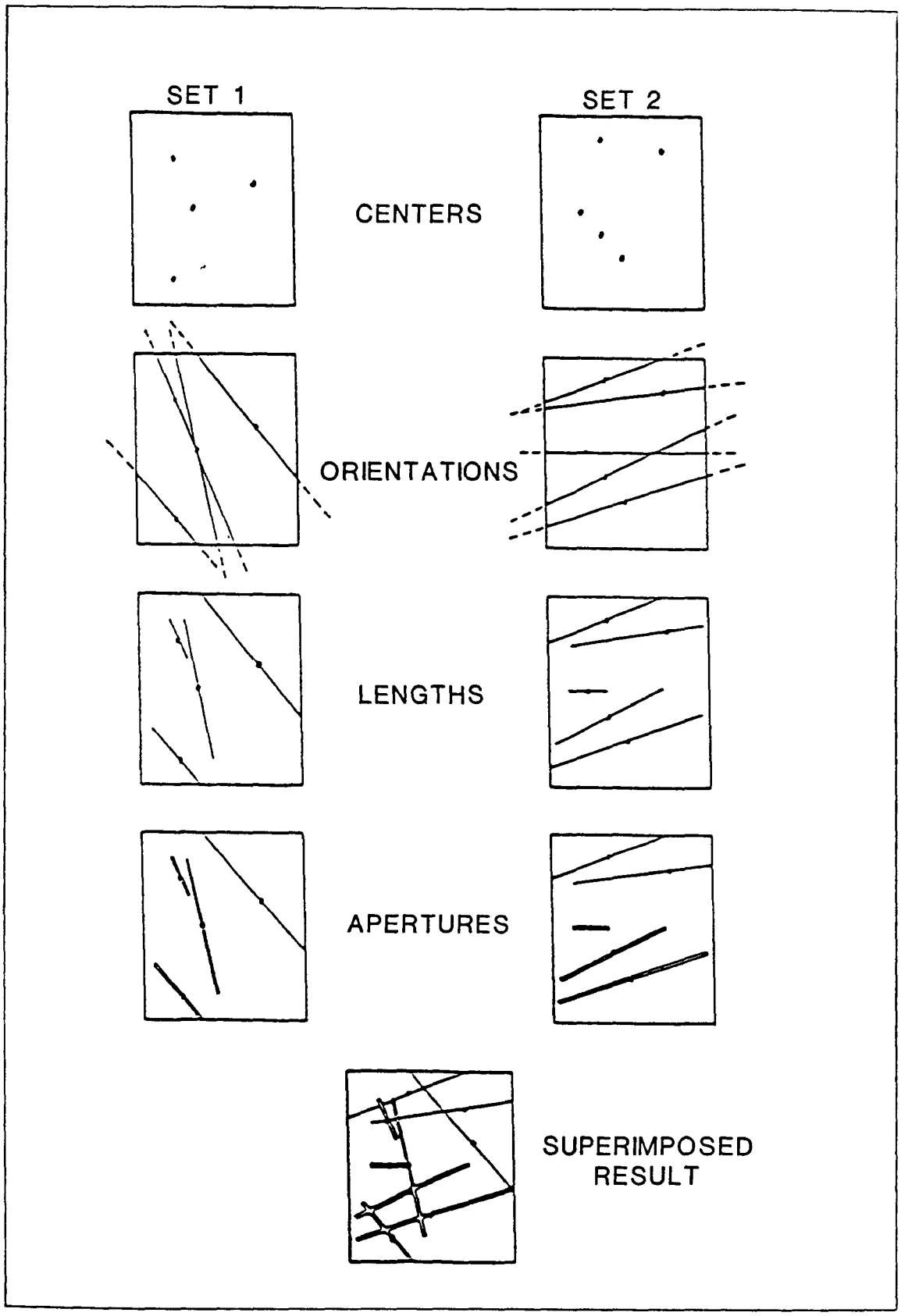


Fig. 26. Generation of a fracture network (after Long and Billaux 1986).

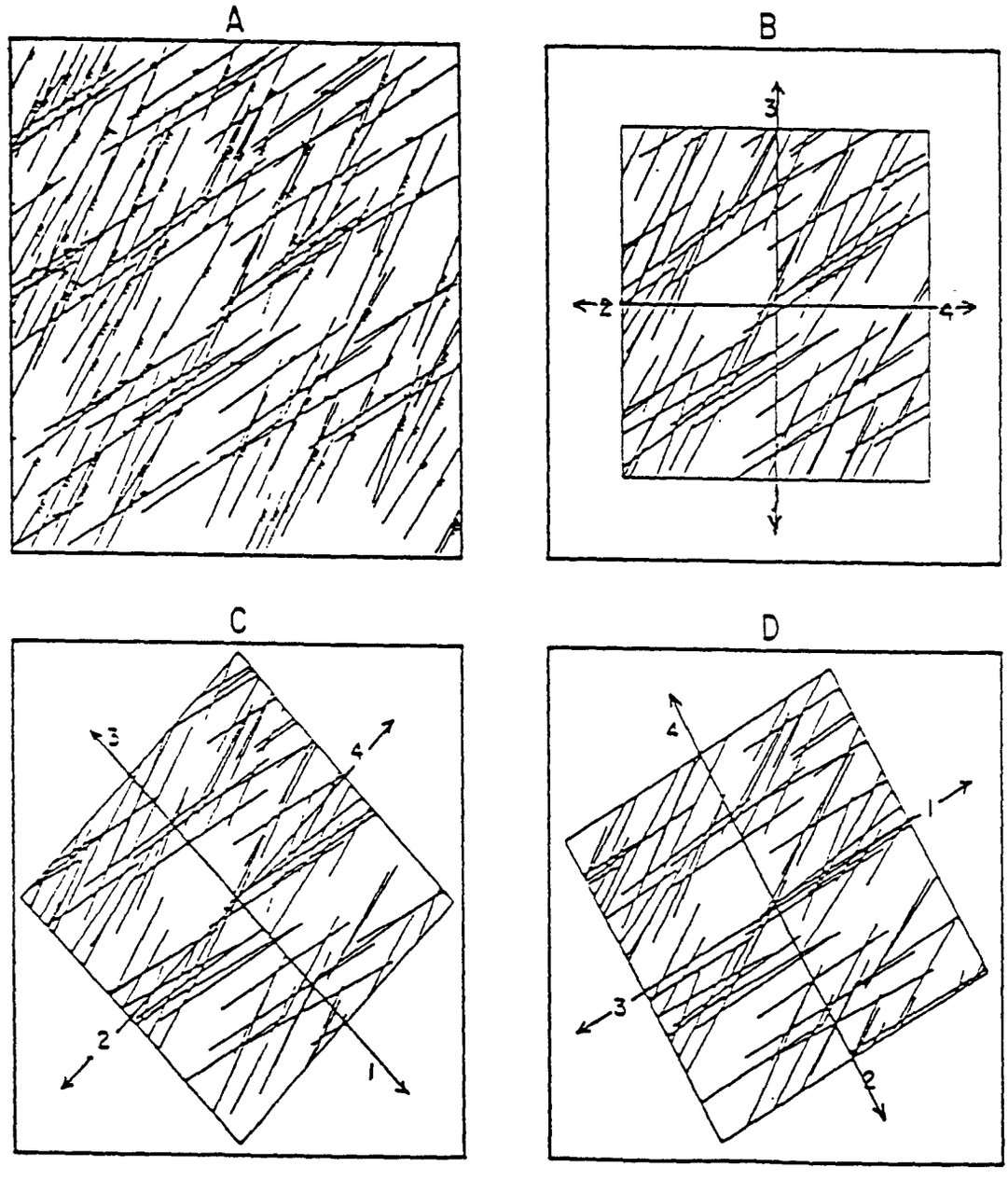


Fig. 27. Relationship between directional fracture properties and orientation of observation or modeling grid (after Long and Billaux 1986).

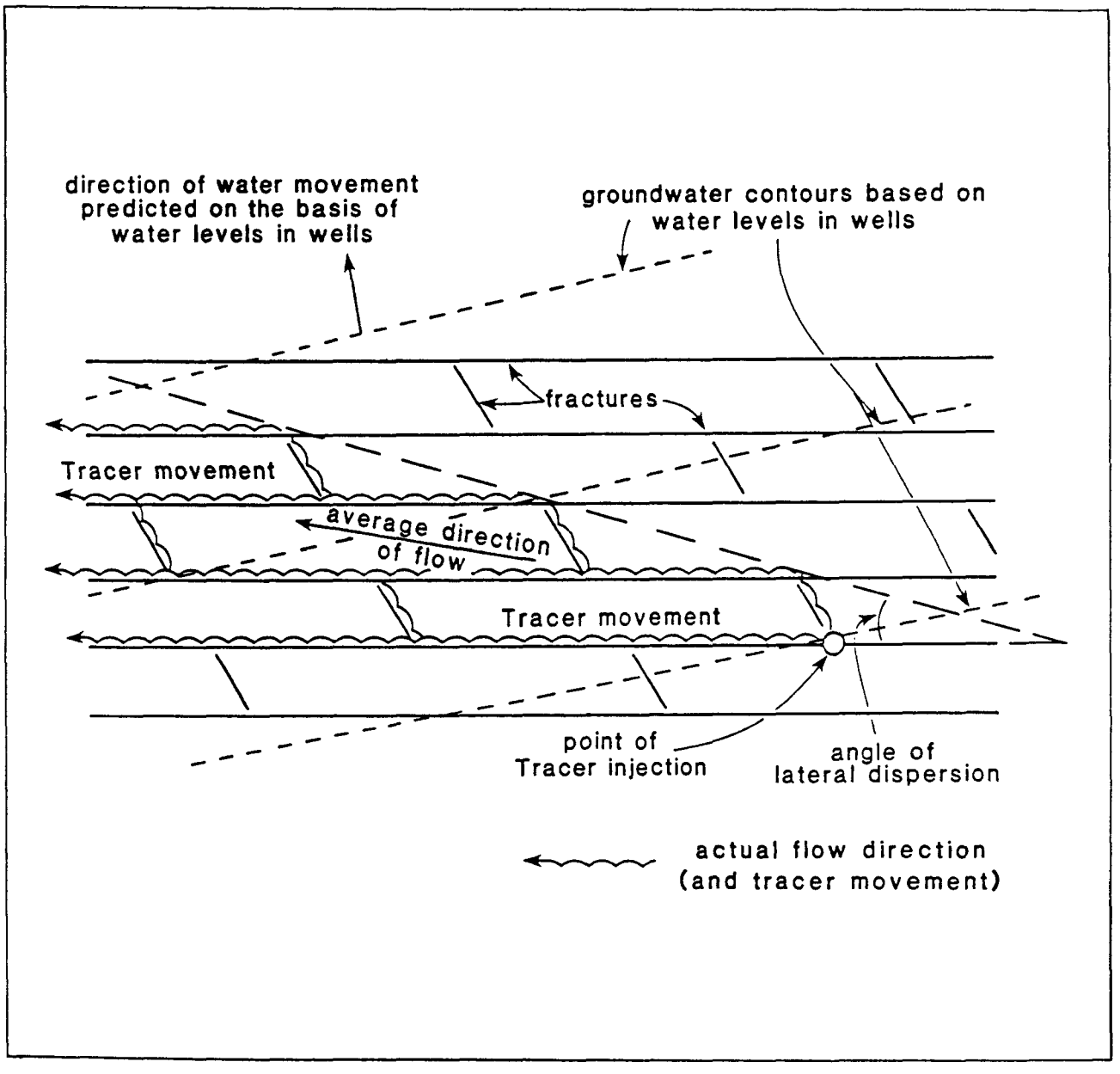


Fig. 28. Two-dimensional fracture pattern and its influence on average flow direction versus actual flow direction (after Davis and Dewiest 1966).

In porous media, the size, shape, and degree of interconnection of the pores regulate the flow rate. The scale of these pores is small and for most purposes the medium may be treated as a continuum in which macroscopic flow properties are considered without regard to the actual flow paths of the individual fluid particles. In a fractured rock, however, the scale of the pores (e.g., fracture space) can be large enough that the continuum approach is not always appropriate, although often used by applying an equivalent porous media concept. In such cases, the network of individual fractures must be analyzed to understand macroscopic flow and transport properties (Endo and Witherspoon 1985).

Flow in relatively large fissures requires a discrete fracture conceptualization where the flow within individual fractures is modeled directly as flow in an interconnected network of channels. The lack of precise information on the configuration of fractures often leads to the necessity of stochastic representation of fracture geometry and distribution (Streile and Simmons 1986).

It should be noted that in unsaturated fractured porous rock, based on capillarity and free energy considerations, moisture tends to accumulate in the porous matrix and only if the flux exceeds the matrix capacity moisture will move in the fractures.

The velocities in large fissures can be relatively high, sometimes causing turbulent flow conditions. The effects of turbulent flow are pore pressures in excess of those resulting from laminar Darcian flow (Elsworth et al. 1985). As mentioned, conventional porous media concepts may not be appropriate. However, the concept of equivalent porous medium is often used for both continuous and discontinuous fracture systems. This approach is based on the observation that the more intersections between fractures present in a fracture network, the more the system is likely to behave as a porous medium (Long and Witherspoon 1985). Conditions for equivalent porous medium behavior for fluid flow in fracture networks have been discussed by Long (1983). Endo and Witherspoon (1985) presented a technique for evaluating porous medium equivalence for the ratio of fluid flux to mean transport velocity, termed hydraulic effective porosity. It should be noted that a system that behaves as a continuum for fluid flux may not behave like a continuum for mechanical transport.

When fractures or solution channels are primarily developed in a single direction, the rock will be strongly anisotropic for flow. The direction of the groundwater flow cannot be predicted by simply drawing orthogonal lines to the groundwater level contours derived for the equivalent porous media. Sometimes, groundwater flow might occur almost parallel to such groundwater level contours (Davis and DeWiest 1966). Figure 28 shows an example of anisotropy in two-dimensional flow in which the head drop in all channels is proportional to the length of the channel.

The fluid flow in a fracture will vary in a parabolic fashion across the fracture (aperture = 2b) from a value of zero at the walls to a maximum at the center of the fracture. This variation is due to the viscous nature of the fluid and the resistance between fluid and fracture wall (Sudicky 1987, pers. comm.) (Figure 29). Advection computations are generally based on the average velocity in the fracture.

Hydraulic conductivity used in the Darcy equation as applied to fractures, is based on a hypothetical fracture geometry such as a parallel plate concept (Figure 29). In reality, the aperture of the fracture might vary significantly over the length of the fracture (Figure 30). To account for such a rough-walled fracture system, the constant value of the aperture can be replaced by a statistical average, based on a schematic asperity model (Figure 30). If only flow in the fracture itself is present, porosity is unity.

In the last ten years research has been focused on determining the factors that control the flow of fluids in fractured rocks. It has been shown that if enough details of the fracture system geometry can be obtained, it is possible to deduce a great deal about the flow properties of the system (Witherspoon et al. 1987). However, the field data necessary to characterize the fracture geometry are not commonly available. An extensive discussion regarding field techniques for characterization of fractured rock systems can be found in Nelson (1985).

Transport in Fractured Media

Contaminant and heat transport in fractured rock formations is governed by the same processes as in granular media: advection, mechanical dispersion, molecular diffusion, and chemical and biochemical reactions and in the case of heat transport, conduction. However, there are some notorious differences in the effects that fractured media can have on these processes due to the need for a detailed description of the fluid velocities, the sparseness of the flow channels, their unequal distribution through the rock media, and in porous rode the interaction between the fluid in the fractures and in the rock matrix. These effects are especially noticeable in observing dispersion and diffusion processes (Schwartz et al. 1983, Sudicky et al. 1985).

Although for the study of the head distrbution in a fractured system the calculation of fluxes is sufficient, for simulation of solute and heat transport the velocity distribution need to be known in detail. The velocities are determined by the active porosity (that part of the pore space in which the fluid movement takes place), which is often much smaller than the total porosity.

Mechanical dispersion in a single fracture consists of longitudinal dispersion only. Fracture width is generally too small to show any significant variation in the distribution of mass across the fracture. A major contributor to macroscopic dispersion in fractured media is the geometry of the network of interconnected discontinuous fractures (Smith and Schwartz 1984). The geometry directly determines the variability of the fluid velocity and the average path length through the interconnecting fractures. In general, the velocities in fractured rock are not normally distributed, precluding the use of a Gaussian dispersion model. Macroscopic dispersion is further complicated by local mixing at the connection between fractures.

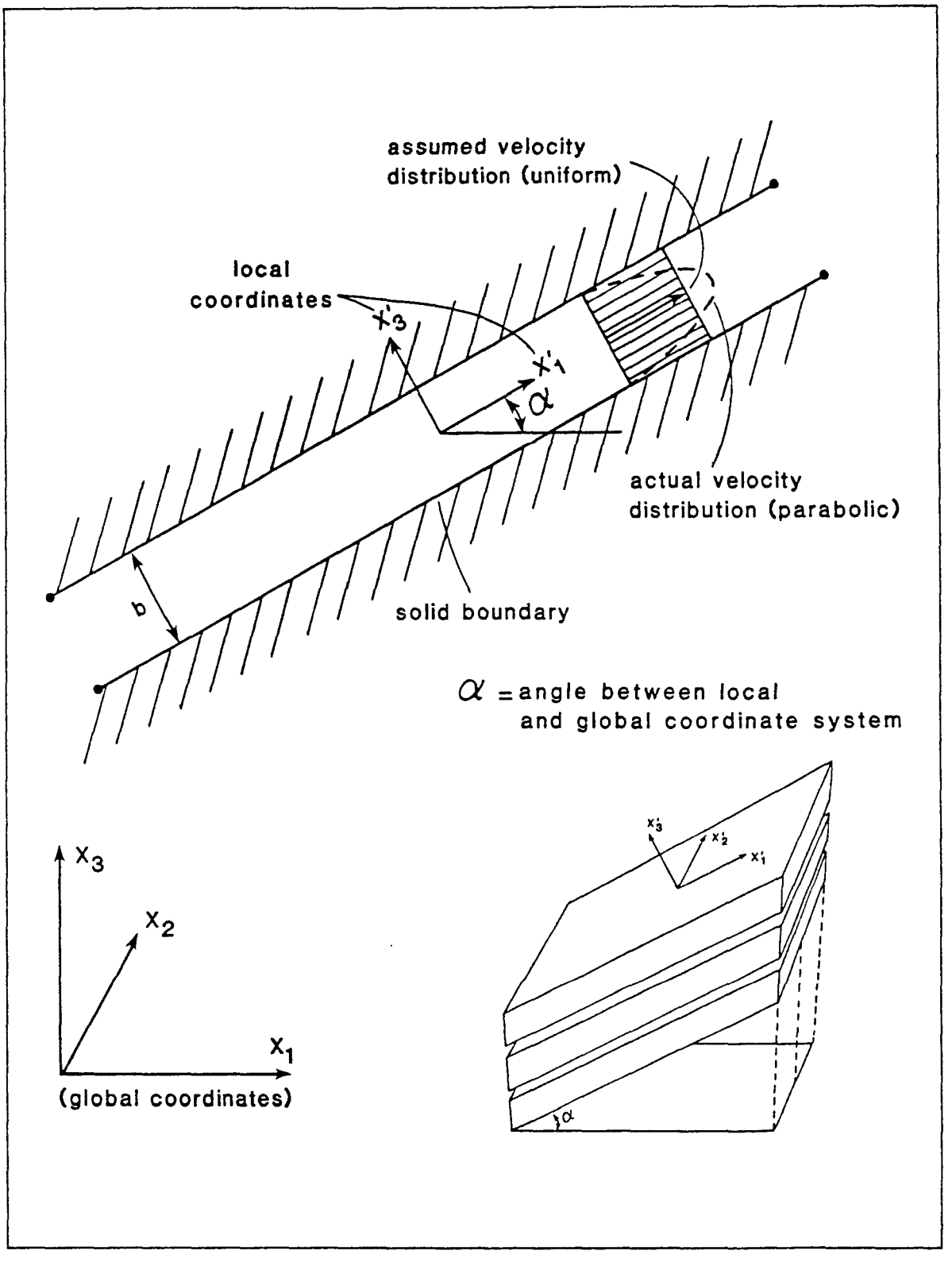


Fig. 29. Laminar flow in a fracture element bounded by two parallel planes (after Huyakorn and Pinder 1983; Huyakorn et al. 1987).

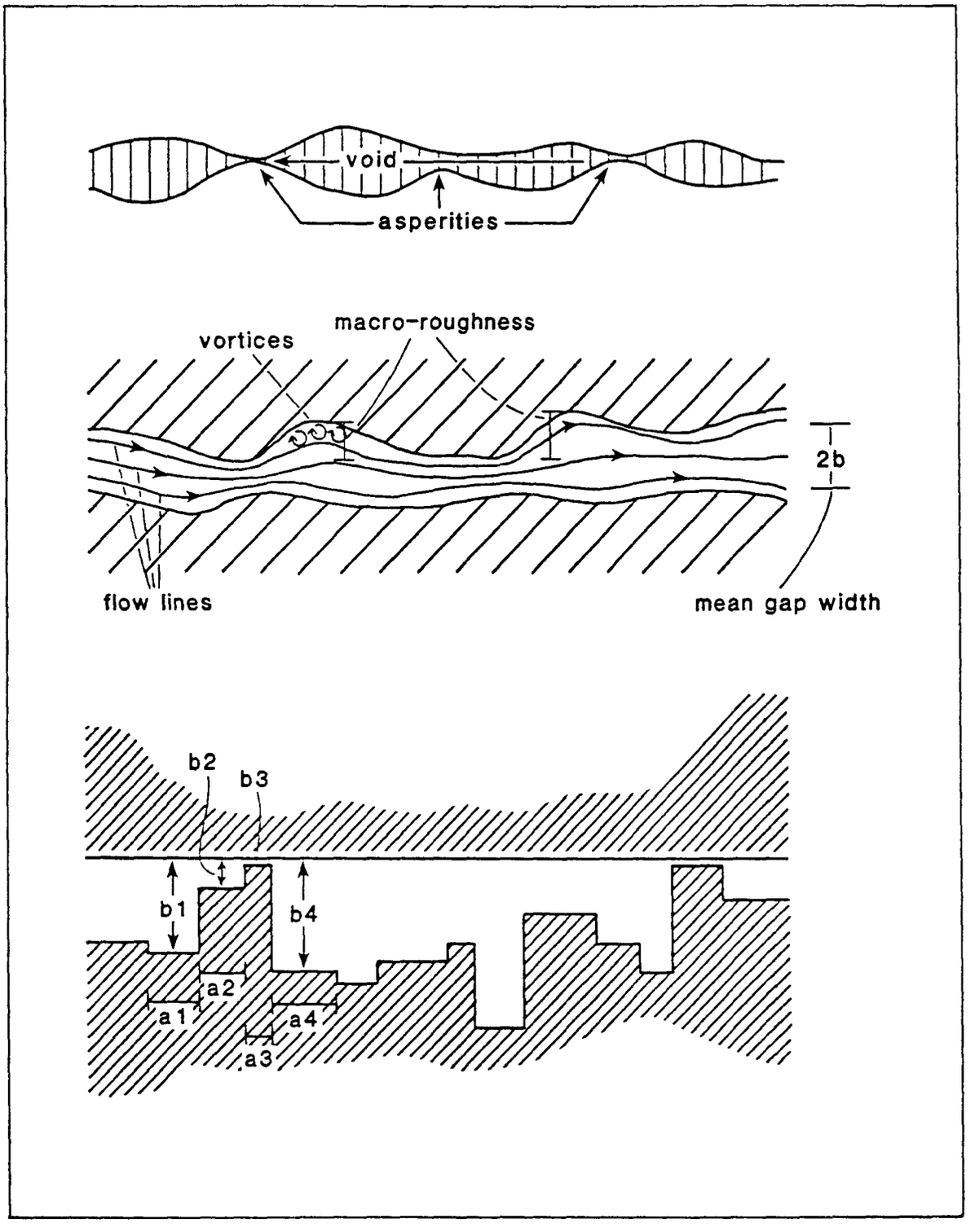


Fig. 30. Geometry and schematization of a single fracture (after Elsworth et al. 1985).

Anderson (1984) concluded that (1) a significant retardation mechanism for pollutant transport in fractures is diffusion of the contaminants into the pores of the rock matrix; and (2) an acceleration mechanism for low-velocity flow in fractures is dispersion within the water phase. Little is known, however, about the magnitude of the roughness of a fracture. Difficulties in describing the geometry and hydraulic characteristics of fractured rock in the field are the major delays in model development and testing.

In dual porosity systems contaminants diffuse from the main fractures into and out of micropores and dead-end fractures systems (Figures 31 and 32). They penetrate the porous rock from the fracture surfaces, resulting in considerable broadening of the zone active in transporting contaminants as compared with transport through equivalent porous media. Unless the source release occurs over a very long period of time, the resulting broadening of the zone of contamination can considerably reduce the peak contaminant concentration, such as in the case of the release of a contaminant slug (Figure 33).

Flow in fractured porous media, which is a combination of flow in fractures and flow in porous media, can result in transient chemical concentration gradients between the water in fractures and pores (Cherry et al. 1984). Although the bulk of the flow occurs in the fractures, diffusion of trace organics and other chemicals into and out of the porous matrix can have a strong influence on contaminant behavior (Tang et al. 1981, Grisak and Pickens 1981). This is caused in part by the fractured surfaces that come into contact with the flow. Pollutants must come into contact with media surfaces before chemical interactions, such as adsorption, may occur. Porous media may also contain organic matter, which enters into reactions (Kincaid and Mitchell 1986).

Cherry et al. (1984) report that the chemical reactions occurring during contaminant transport can be significantly different in porous media and fractured rock (or fractured, fine-grained, nonindurated porous media). Advection theory and the isotherm approach to predictive transport modeling have been specifically developed for porous media. Measurement of adsorption parameters for predictive modeling of fracture flow in nonporous rock (such as granite) is very difficult. The distribution coefficient must be defined in terms of effective surface area of reaction in the fractures instead of in terms of the mass of solids, as is done for porous media. Cherry et al. (1984) state that few attempts have been made to determine these properties for undisturbed surfaces or to validate predictive models under field conditions.

Analysis of dispersion and chemical processes for contaminant transport in fractured rock, such as shale, granite, basalt, or salt, are in the preliminary stage of development (Anderson 1984, Cherry et al. 1984). This type of analysis may be needed where deep-well injection of hazardous wastes can result in pollutant transport to the biosphere. Clay, which is also susceptible to fracturing, is used as a disposal medium for municipal, industrial, and low-level radioactive wastes. Therefore, hazardous chemical movement caused by the possible increase of flow velocities in fractured porous media over that seen in a uniformly porous medium is of major concern (Kincaid and Mitchell 1986).

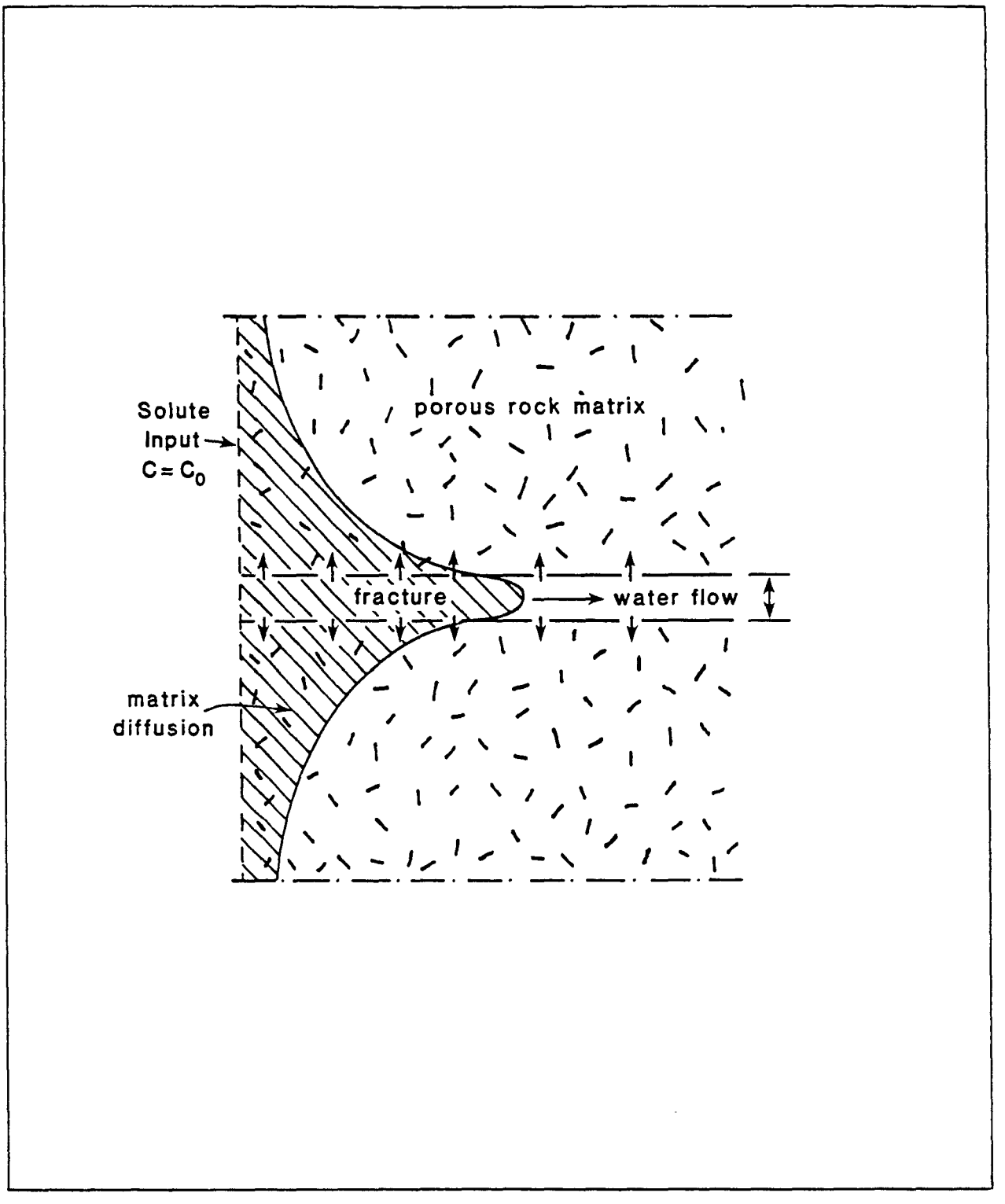


Fig. 31. Diffusion from fracture into porous matrix for continuous source (after Huyakorn et al. 1987).

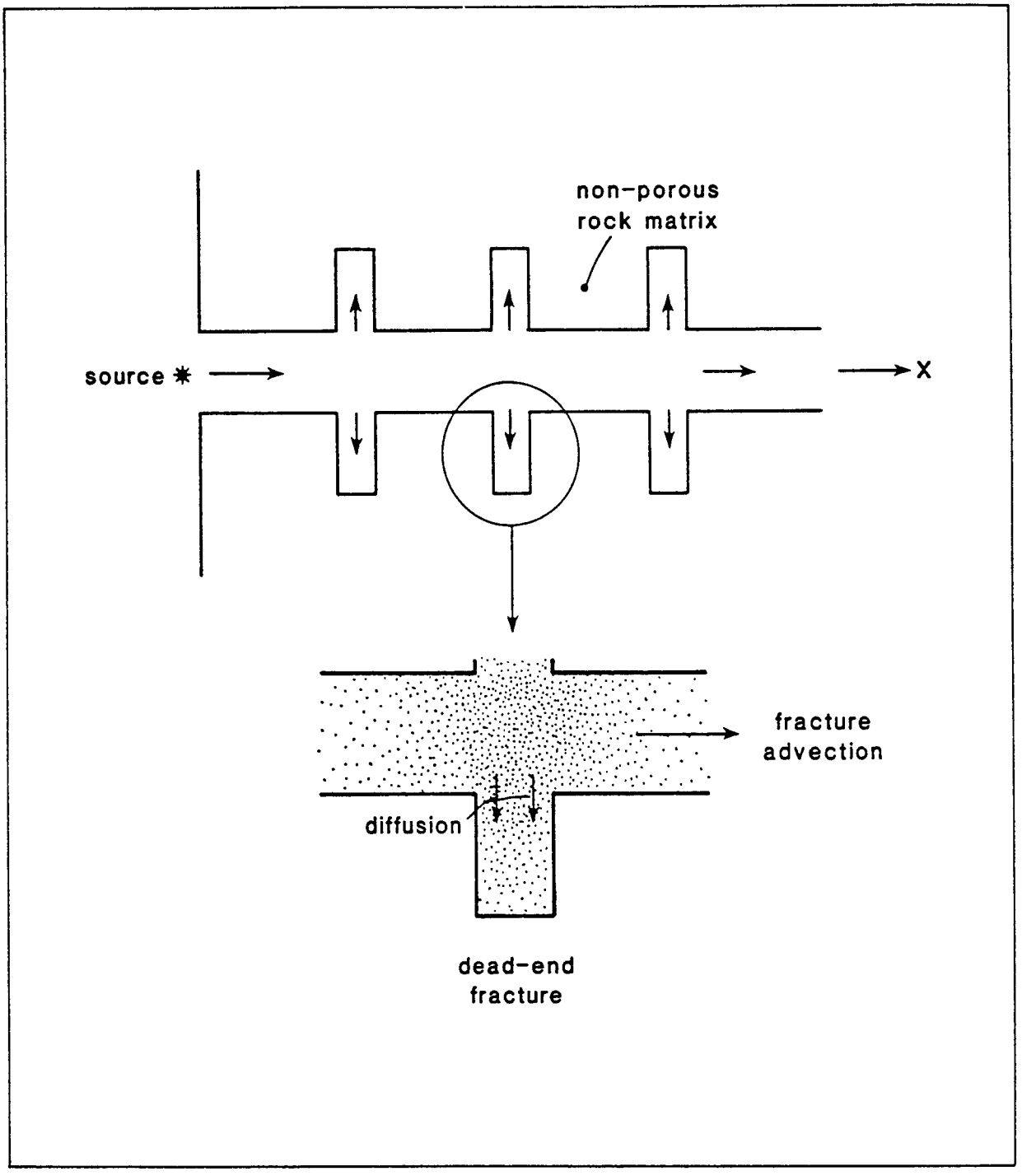


Fig. 32. Diffusion from active fracture into dead-end pores and fractures.

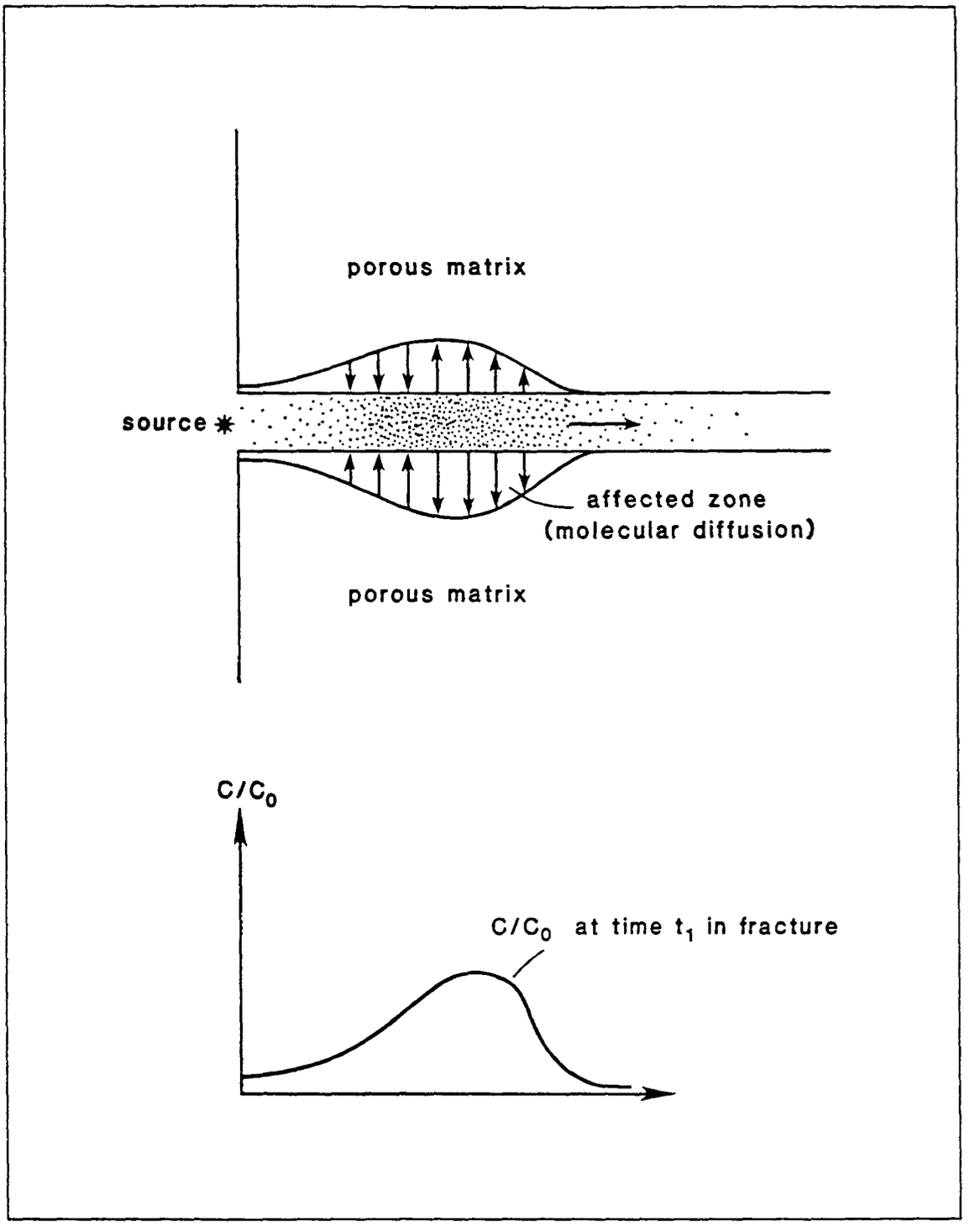


Fig. 33. Diffusion into and out of porous matrix for a slug source.

Flow and Transport Models for Fractured Rock

Recent developments in mathematical models of flow in fractures have been based on the concept of a dual porosity medium (Grisak and Pickens 1981, Huyakorn 1987). A few mathematical models exist for modeling flow and transport in saturated fractured and dual porosity media. Various analytical solutions for solute transport in simple fractured systems are brought together in the CRACK package (Sudicky 1986). These solutions include transport in a single fracture with matrix diffusion (but without dispersion along fracture axis), transport in a system of parallel fractures including matrix diffusion, and transport in a single fracture with matrix diffusion and radial diverging flow. A typical numerical model for flow and transport of heat and nonconservative solutes in fractured rock is the TRAFRAP-WT code developed for the International Ground Water Modeling Center (Huyakorn 1987) This code is a two-dimensional finite-element code capable of treating both confined and water table aquifers. Fractured rock can be modeled as a system of discrete fractures or as a double porosity system by overlaying the two-dimensional element grid for the porous medium with one-dimensional line elements representing discrete fractures (Figure 34). This approach requires that the geometry of the fracture system is defined on an appropriate scale.

An example of a finite difference model designed to handle solute and heat transport in fractured porous media is the FRASCL code (Fractured Media - Advanced Continuous Simulation Language) developed at the Idaho National Engineering Laboratory (Miller 1983, Clemo and Hull 1986). This code simulates the fractured system as discrete parallel sided channels in the porous matrix. As with the TRAFRAP model this code allows for diffusion of chemical compounds from the liquid in the fractures into the matrix blocks. The porous aquifer is defined by a rectangular finite difference grid of unit thickness. Fractures connect any two adjacent nodes, vertically, horizontally or diagonally, with a maximum of eight fractures converging at a single node. As in TRAFRAP, fractures can have any configuration of length, angle, and start and termination location, constrained only by the connectivity criterion mentioned. Aperture is constant between two directly connected nodes, but for the same fracture can change in the grid section being the fracture's continuation between the next set of nodes. These and other codes that are capable to simulate fractured systems are listed in Appendix F.

Another example of the dual porosity concept used in transport modeling in fractured rock is the MINC (Multiple INteracting Continua) method developed by Pruess and Narasimhan (1982a,b). In the double porosity approach the fractured porous reservoir is partitioned into (1) a primary porosity, which consists of small pores in the rock matrix; and (2) a secondary porosity, consisting of fractures and joints (Pruess 1983). Each of the two porosities is treated as a continuum, whose properties can be characterized by means of the traditional porous medium properties, i.e., permeability, porosity, and compressibility. The porous matrix is divided in a series of interbedded subsystems such that there is thermodynamic equilibrium in all volume elements at all time (Figures 35, 36 and 37). The MINC method treats the interporosity flow (i.e., the exchange between porous matrix and fracture system e.g., diffusion of solutes from the fractures into the porous matrix) as a series of mass exchanges between the nested subsystems. Global flow occurs only through the network of fractures (Figure 38). An implementation of the MINC concept in simulating transport of solutes is found in Narasimhan and Pruess (1987)

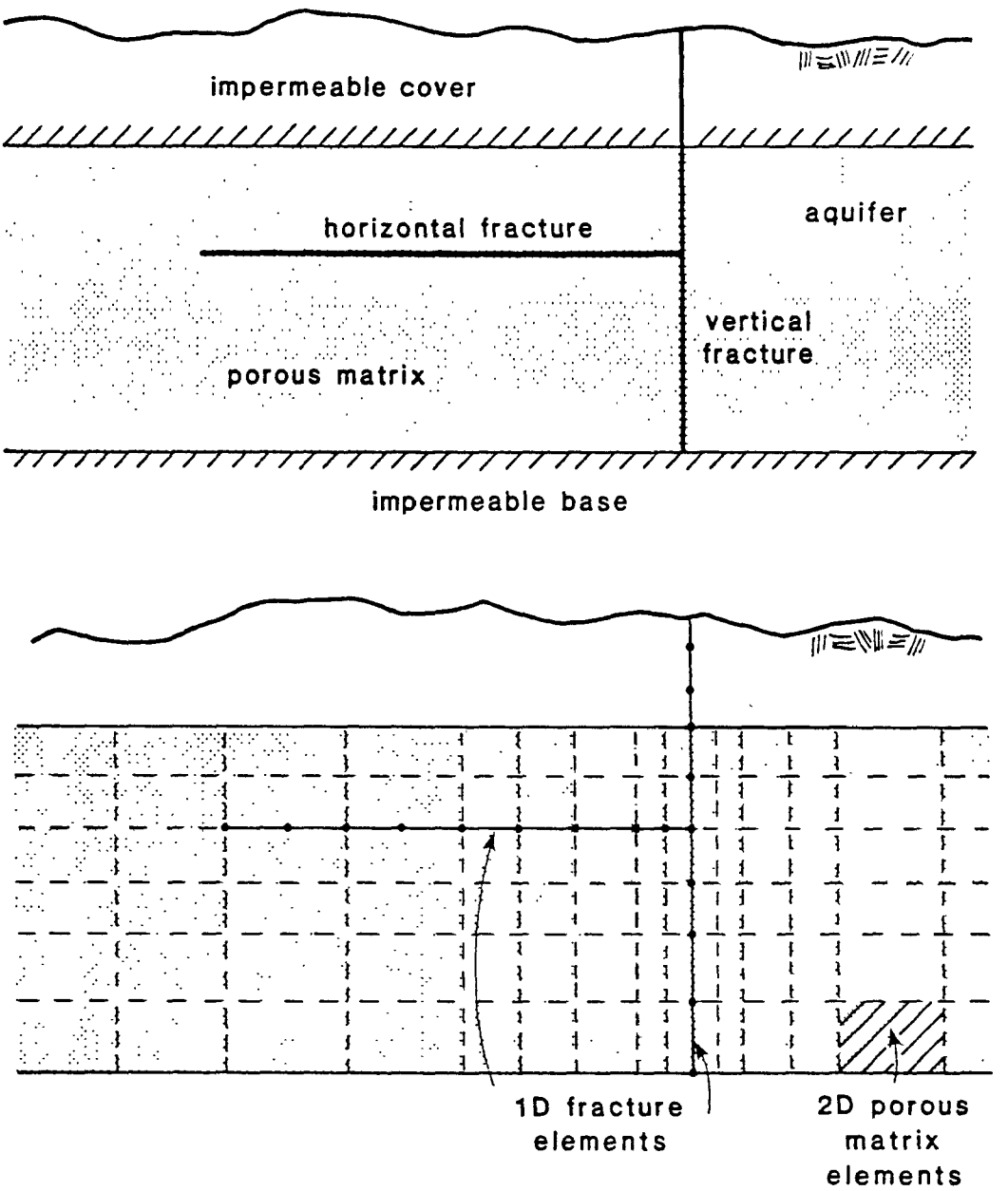


Fig. 34. Treatment of system with intersecting discrete fractures, using TRAFRAP.WT (after Huyakorn et al. 1987).

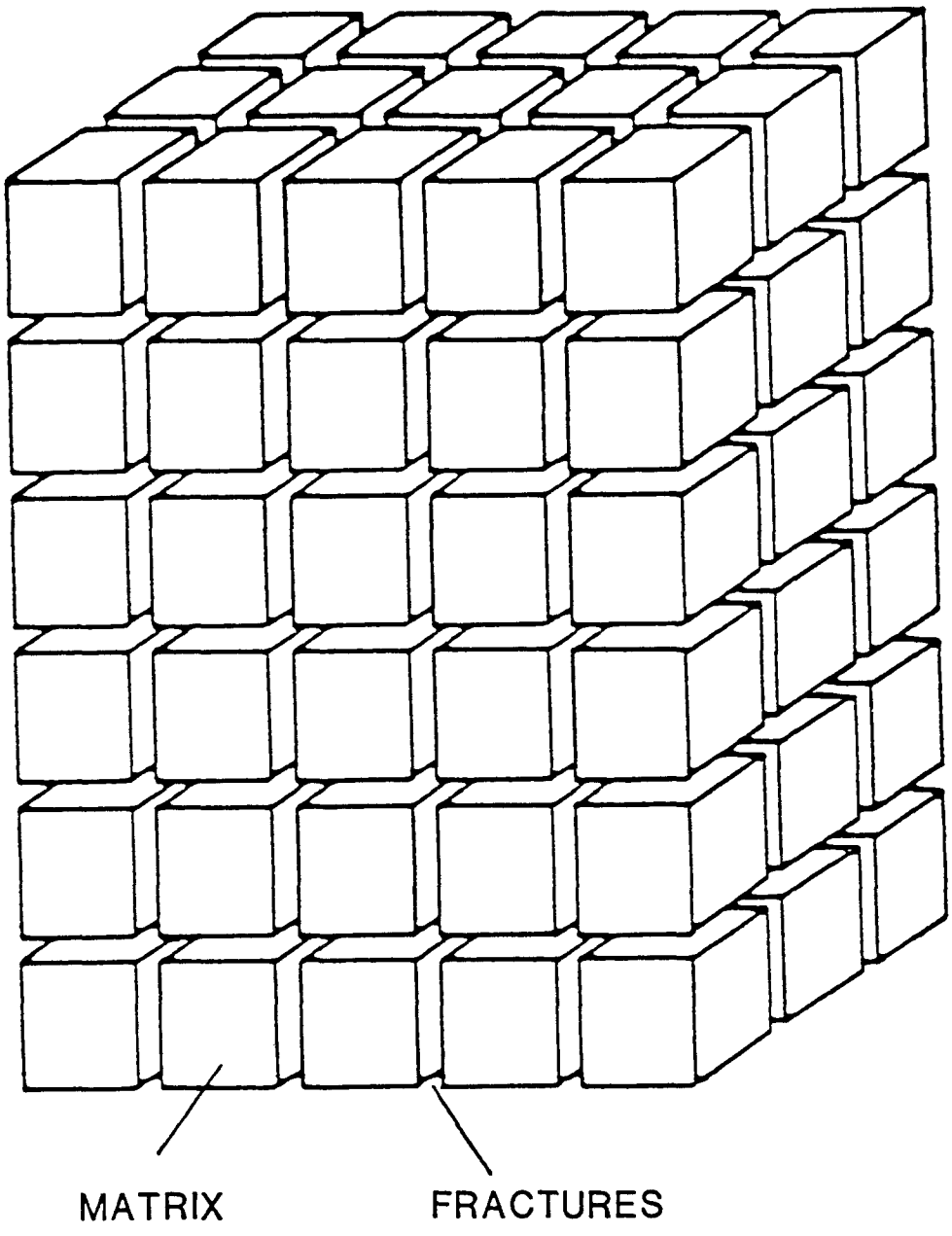


Fig. 35. Idealized model of a fractured porous medium (from Pruess 1983).

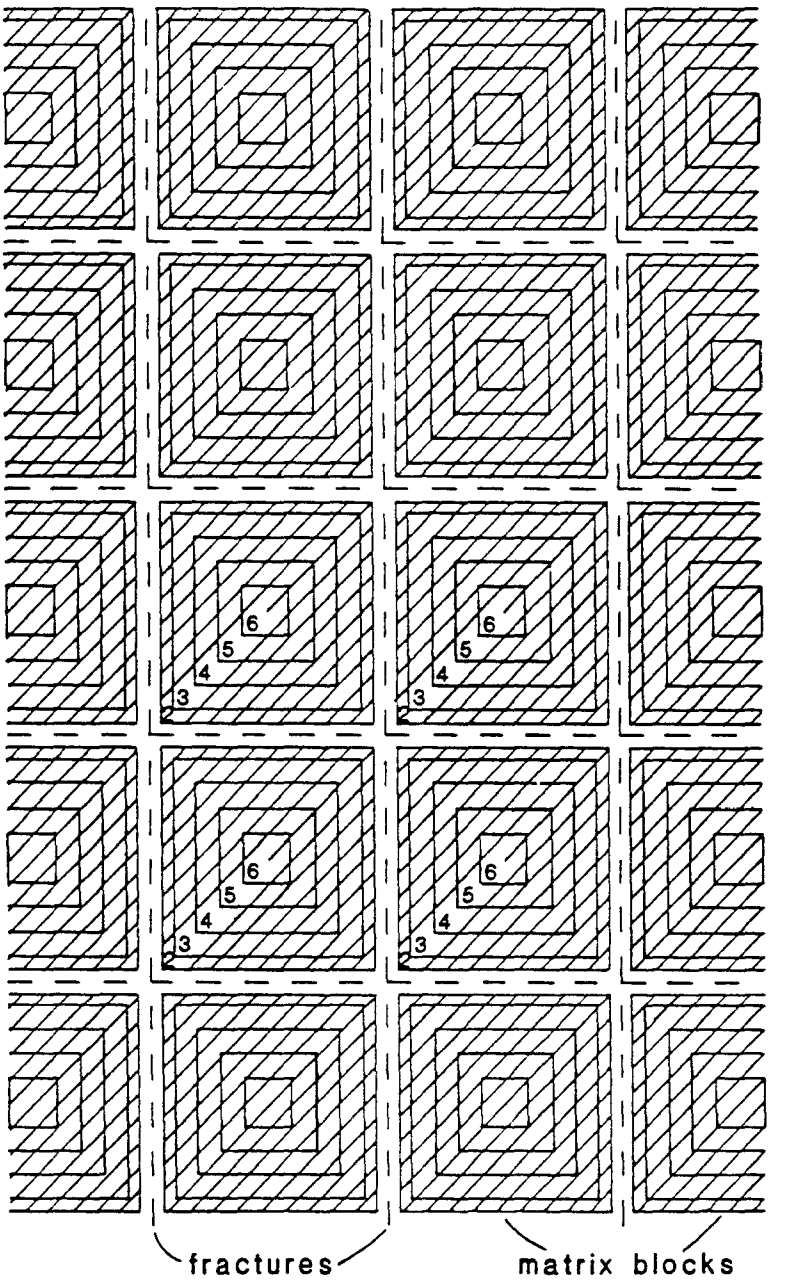


Fig. 36. Basic computational mesh for a fractured porous medium (from Pruess 1983).

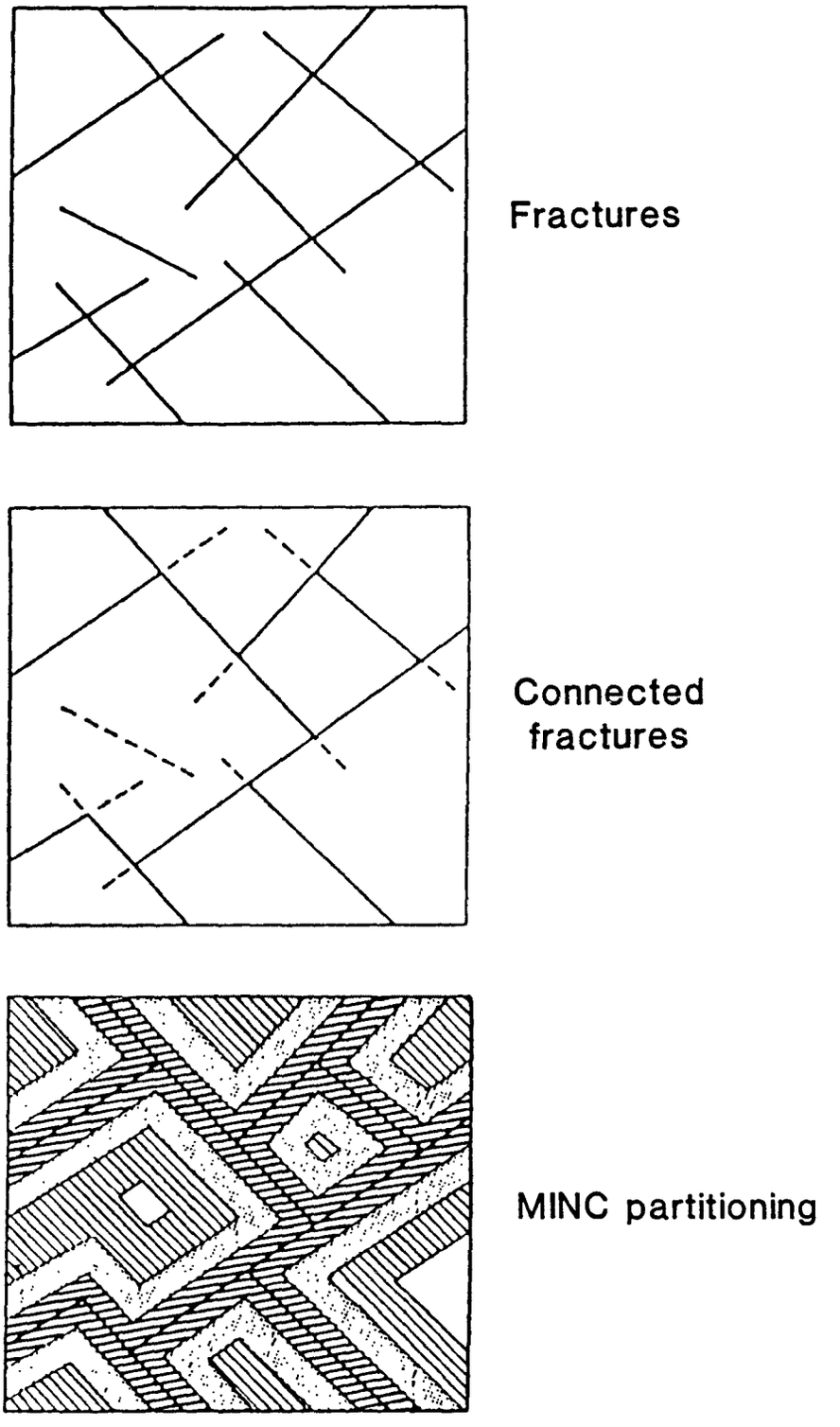


Fig. 37. MINC concept for an arbitrary two-dimensional fracture distribution (from Pruess 1983).

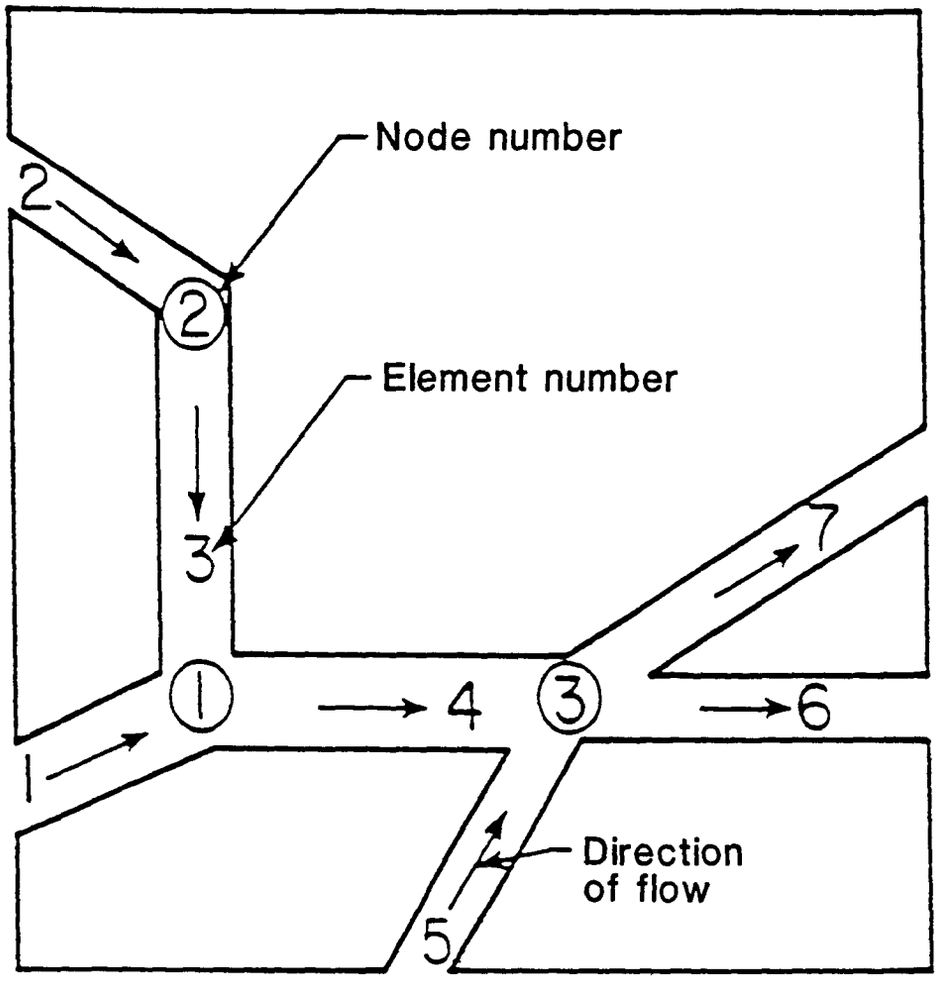


Fig. 38. Network approach in modeling interconnected fracture systems (from Endo et al. 1984).

using the Integral Finite Difference Method (IFDM) for solving the governing equations.

A continuum approach for modeling mass transport in fractured rock based on the application of a particle tracking method is presented by Schwartz and Smith (1988). The physical transport is simulated in terms of velocity and velocity variations using statistics to describe the particle motion in a representative subdomain of the modeled aquifer region (Figures 39 and 40). For each of the particles a trajectory is plotted dependent on the statistic properties of the fracture distribution and the global flow field calculated with a finite element model using triangular elements and linear basis functions. This approach leads to the definition of an equivalent continuum for the fractured medium. Dispersion is accounted for by the variability in flow conditions.

Codes that are well accepted as representing single-phase flow and solute transport through unsaturated fractured media are presently not available. A recent discussion on the state-of-the-art of computer modeling flow and transport through unsaturated fractured rock system can be found in Evans and Nicholson, eds. (1987). While models of single-phase fluid in a porous media are to some extent applicable to multiphase fluids in porous media, no such extension of mathematics and numerical methods can yet be made for applications to fractured media (Kincaid and Mitchell 1986).

As larger fractures often transport a fraction of the solute or heat disappropriately large for its relative pore volume, the presence of such larger fractures requires special attention in modeling. Simulations conducted in a hypothetical fractured porous aquifer with constant overall porosity but varying rate between pore and fracture porosity and with varying distribution of fracture size and interconnectivity demonstrated that good results can be obtained if an adequate active porosity can be determined (Hull and Clemo 1987). Furthermore Hull and Clemo (1987) found that the success rate in the simulations of dual porosity systems is directly influenced by the level to which the most significant discrete fractures are explicitly simulated. It should be noted that in heat transport conduction of heat through the solids is an important additional process that results in a larger area of the aquifer participating in the transport than is the case for solute transport.

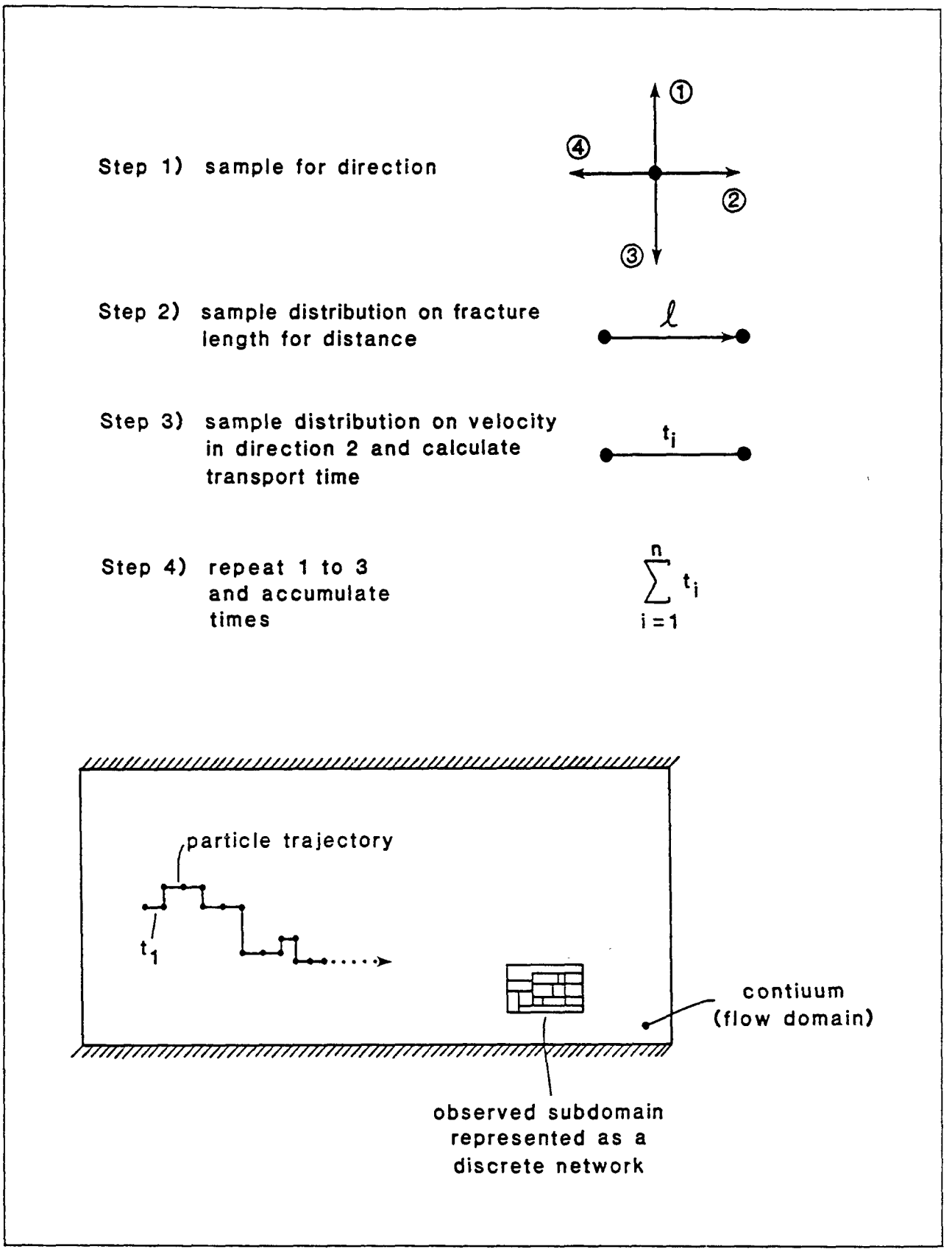


Fig. 39. Simulation of transport in a fracture continuum (from Schwartz and Smith 1988).

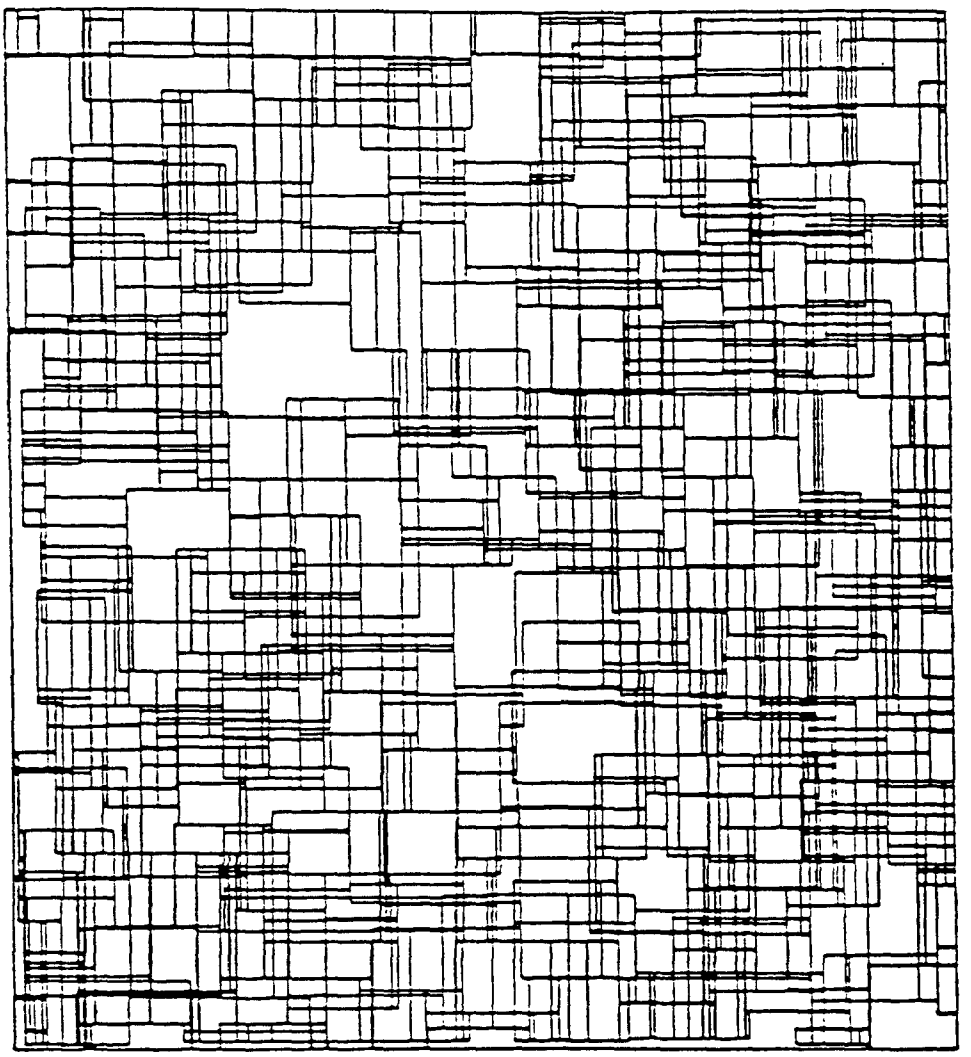


Fig. 40. Combined trajectories of particles simulating random movement in a fractured system (from Schwartz and Smith 1988).

6. QA IN MODELING

THE ROLE OF QUALITY ASSURANCE

To develop effective software and to apply it in analyzing alternative solutions to groundwater problems requires a number of steps, each of which should be taken conscientiously and reviewed carefully. Taking a systematic, well-defined, and controlled approach to all steps of the model development and application process is essential for the success of modeling in water resource management. Quality Assurance (QA) provides the mechanisms and framework to ensure that decisions are based on the best available data and (modeling-based) analyses. This does not imply that analyses based on the use of quality-assured models and modeling projects are guaranteed to provide correct answers.

Many modeling studies are performed without adequate QA arrangements in place. QA plans are often lacking and formal QA assessment is frequently postponed until the project reaches its final stage (van der Heijde and Park 1986). This is especially true for studies where models are applied to site-specific problems. In contrast, policies based on modeling assessments often affect large constituencies and thus are more thoroughly scrutinized before they are adopted. Increasingly, financial and criminal liability require modelers to implement rigorous QA procedures in all stages of the projects.

Frequently mentioned reasons for deficiencies in QA are lack of specifications from management with respect to the level of analysis required for decision making; shortage of time, budget, and experienced staff; unfamiliarity with QA procedures; and reluctance to accept additional administrative duties (van der Heijde and Park 1986).

Program managers in regulatory agencies play a crucial role in QA, as their decisions rest on the quality of environmental data and data analysis. They are in a unique position to specify the quality of the environmental data and the level of problem-solving data analysis required, and to provide sufficient resources to assure an adequate level of QA.

To alleviate the lack of information on QA in groundwater modeling, this section provides background information on QA and discusses the role of QA in groundwater modeling. It presents a comprehensive set of procedures together forming a functional quality-assured modeling methodology. It is written from the perspective of the model user and the decision maker in need of technical information on which to base decisions. Various standards and guidances applicable to groundwater modeling are given and areas are identified where additional research and regulation is required. The section is divided in three parts: (1) model development, (2) model application, and (3) model selection.

It should be noted that relatively little has been published in the open literature on QA in software application, as compared with QA in software development.

DEFINITIONS

Quality assurance in groundwater modeling is the procedural and operational framework put in place by the organization managing the modeling study, to assure technically and scientifically adequate execution of all project tasks included in the study, and to assure that all modeling-based analysis is verifiable and defensible (Taylor 1985). QA in groundwater modeling is crucial to both model development and model application and should be an integral part of project planning and be applied to all phases of the modeling process.

The two major elements of quality assurance are quality control (QC) and quality assessment. Quality control refers to the procedures that ensure the quality of the final product. These procedures include the use of appropriate methodology, adequate validation, and proper usage of the selected methods and models.

To monitor the implementation of quality control procedures and to evaluate the quality of the studies, quality assessment is applied (van der Heijde 1987a). It consists of two elements: auditing and technical review. Audits are administrative procedures designed to assess the degree of compliance with QA requirements, commensurate with the level of QA prescribed for the project. Compliance is measured in terms of traceability of records, accountability (approvals from responsible staff), and fulfillment of commitments described in the QA plan of a project. Technical review consists of independent evaluation of the technical and scientific basis of a project and the usefulness of its results. In groundwater modeling this latter form of quality assessment is rather common.

There is a significant difference between software quality assurance (SQA) and hardware QA (Bryant and Wilburn 1987). Therefor, special SQA procedures need to be established and detailed. It should be noted also, that major differences exist between data QA (e.g., EPA 1986b), software QA and model application QA.

THE QA PLAN

At the beginning of a model development or application project, a project plan should be made containing a complete set of QA procedures, sometimes called the QA plan. These QA procedures comprise a list of the measures required to achieve prescribed quality objectives. The QA plan needs approval before initiation of technical work. Major elements of such a QA section of the project plan or QA plan are:

- Formulation of QA objectives and required quality level in terms of validity, uncertainty, accuracy, completeness, and comparability
- Development of operational procedures and standards for performing adequate software development and modeling studies
- Establishing a paper trail for QA activities in order to document that standards of quality have been maintained

- Internal and external auditing and review procedures.

The QA plan should also specify individual responsibilities for achieving these goals, describe the technical chain-of-command within the project organization, and outline procedures for remedial or corrective action in case problems are detected in the quality assessment stage.

Many modeling studies are performed without adequate QA arrangements in place. A formal QA plan is often lacking and extensive QA assessment is frequently postponed until the project reaches its final stage (van der Heijde and Park 1986). This is especially true for studies where models are applied to solve site-specific problems. In contrast, policies based on modeling assessments often affect large constituencies and thus are more thoroughly scrutinized before they are adopted. Increasingly, financial and criminal liability require modelers to implement rigorous QA procedures in all stages of the projects.

QA IN CODE DEVELOPMENT AND MAINTENANCE

Software quality assurance (SQA) consists of the application of procedures, techniques, and tools throughout the software life cycle, to ensure that the products conform to prespecified requirements (Bryant and Wilburn 1987). This requires that in the initial stage of the software development project appropriate SQA procedures (e.g., developing a QA plan, record keeping, establishing a project QA organization), techniques (e.g., auditing, design inspection, code inspection, error-prone analysis, functional testing, logical testing, path testing, reviewing, walk-throughs), and tools (e.g., text-editors, software debuggers, source code comparitors, language processors) need to be identified and the software design criteria be determined. Many current groundwater modeling codes have not been subject to such a rigorous SQA approach. Ideally, SQA should be applied to all codes currently in use and yet-to-be-developed codes.

The use of the software life cycle concept has proven successful in determining the QA requirements of the development, use, and operation of software systems (Bryant and Wilburn 1987). The software development life cycle consists of three major phases: the initiation phase, the development phase, and the operation phase (NBS 1976). In the initiation phase the objectives and requirements for software are defined, and feasibility studies and cost-benefit analysis performed. In the development phase software and documentation requirements are determined, program design formulated, coding implemented, and code testing performed. During this phase, and parallel with program design and coding, the user's manual, the operations manual, and the program maintenance manual should be written.

In the operation phase the software is used for the purpose for which it has been designed. During this phase the software is maintained, evaluated regularly, and changed as additional requirements are identified. When maintenance is no longer justified (e.g., because of changes in computer environments used, changes in operational requirements, or changes in software design objectives), the end of the software life cycle is reached. A detailed discussion of the QA requirements for each of these software life cycle phases is given by Bryant and Wilburn (1987).

The most important QA procedures in code development and maintenance are (van der Heijde 1987a):

- Documentation of code development (record keeping)
- Verification of program structure and coding
- Validation of complete software product (model validation)
- Documentation of code characteristics, capabilities and use
- Scientific and technical reviews
- Administrative auditing.

It should be noted that code testing is generally considered to encompass verification and validation of the model (Adrion et al. 1982).

To evaluate groundwater models in a systematic and consistent manner, the International Ground Water Modeling Center (IGWMC) has developed a model review, verification, and validation procedure (van der Heijde et al. 1985b) which follows in part the testing approach taken by Nicholson et al. (1987).

If any modifications are made to the model coding for a specific problem, the code should be tested again; all QA procedures for model development should again be applied, including accurate record keeping and reporting. All new input and output files should be saved for inspection and possible reuse.

A detailed discussion of QA requirements for record keeping, program structure and code verification, model validation, and software documentation, and the role of scientific and technical reviews is given in the report of the Committee on Groundwater Modeling Assessment (NRC 1988, in preparation).

QA IN CODE APPLICATION

Quality assurance in model application studies follows the same pattern discussed for model development projects, and consists of using appropriate data, data analysis procedures, modeling methodology and technology, administrative procedures, and auditing. To a large extent, the quality of a modeling study is determined by the expertise of the modeling and quality assessment teams.

Quality assurance in code application should address all facets of the modeling process. It should address such issues as:

- Correct and clear formulation of problems to be solved
- Project description and objectives
- Type of modeling approach to the project
- Is modeling the best available approach and if so, is the selected model appropriate and cost-effective?

- Conceptualization of system and processes, including hydrogeologic framework, boundary conditions, stresses, and controls
- Detailed description of assumptions and simplifications, both explicit and implicit (to be subject to critical peer review)
- Data acquisition and interpretation (including discussion of error and inaccuracies and of their propagation in the analysis)
- Model selection process and justification
- Model preparation (parameter selection, data entry or reformatting, gridding)
- The validity of the parameter values used in the model application
- Protocols for parameter estimation and model calibration to provide guidance, especially for sensitive parameters
- Level of information in computer output (variables and parameters displayed, formats, layout)
- Identification of calibration goals and evaluation of how well they have been met
- The role of sensitivity analysis
- Post-simulation analysis (including verification of reasonability of results, interpretation of results, uncertainty analysis, and the use of manual or automatic data processing techniques, as for contouring)
- Establishment of appropriate performance targets (e.g., 6-foot head error should be compared with a 20-foot head gradient or drawdown, not with the 250-foot aquifer thickness!); these targets should recognize the limits of the data
- Presentation and documentation of results
- Evaluation of how closely the modeling results answer the questions raised by management.

QA for model application should include complete record keeping of each step of the modeling process. The paper trail for QA should consist of reports and files that include a description of

- Assumptions
- Parameter values and sources
- Boundary and initial conditions
- Nature of grid and grid design justification
- Changes and verification of changes made in code

- Actual input used
- Output of model runs and interpretation
- Validation (or at least calibration) of model.

As is the case with model development QA, all data files, source codes, and executable versions of computer software used in the modeling study should be retained for auditing or post-project reuse (in hard-copy and, at higher levels, in digital form):

- Version of source code used
- Verification input and output
- Validation input and output
- Application input and output.

If any modifications are made to the model coding during code application to a specific problem, the code should be tested again; all QA procedures for model development should again be applied, including accurate record keeping and reporting. All new input and output files should be saved for inspection and possible reuse together with existing files, records, codes, and datasets.

An increasing number of costly decisions are made based in part on the outcome of modeling studies. In the light of major differences noted in comparative studies on model application (e.g., McLaughlin and Johnson 1987, Freyberg 1988) and the general lack of confidence in modeling results, effective quality assurance might go so far as to require the analysis being done by at least two independent modeling teams. In that case, a third team should review and compare the results of both modeling efforts and assess the importance and nature of differences present.

A detailed discussion of QA aspects in model application, including data collection, model formulation, sensitivity analysis, code implementation and execution, and the interpretation of results, is given in the report of the Committee on Groundwater Modeling Assessment (NRC 1988, in preparation).

QA ASSESSMENT

The final stage in quality assurance is quality assessment. Quality assessment consists of two elements: auditing and technical review (van der Heijde 1987a). Audits are procedures designed to assess the degree of compliance with QA requirements, commensurate with the level of QA prescribed for the project. Compliance is measured in terms of traceability of records, accountability (approvals from responsible staff), and fulfillment of commitments in the QA plan. Technical review consists of independent evaluation of the technical and scientific basis of a project and the usefulness of its results.

QA assessment not only involves checking to see if procedures have been applied correctly, but also establishing quantitatively the overall success of the project in meeting its original objectives.

Various phases of quality assessment exist for both model development and application. First is review and testing in case of software development, or review and performing control calculations by the responsible researcher, and sometimes by other staff not involved in the project, or by invited experts from outside the organization. Also to be considered is the quality assessment by the organization for which the project has been carried out. Again, three levels can be distinguished: project or product review or testing by the project officer or project monitor, by technical experts within the funding or controlling organization, and by an external peer review panel (van der Heijde 1987a).

Quality assessment generally takes the form of technical and administrative reviews. Review comments can be presented in the form of a memorandum or report, or as annotations in the margin in a certified copy of the reviewed documents. In case this review should lead to important recommendations for corrective action or additional studies, follow-up activities by the project team, and additional review, need to be arranged and documented.

QA ORGANIZATION STRUCTURE

QA is the responsibility of both the project team (quality control and internal auditing) and the contracting or supervising organization (quality assessment). QA should not drive or manage the direction of a project nor is QA intended to be an after-the-fact filing of technical data.

There are two levels in the QA framework within the organization that carries out a software development or model application study: (1) a permanent organization complete with QA management policies, goals, and objectives, and (2) project QA organization where general QA policies and assignments are detailed towards project objectives. Upper levels of management need to recognize that QA is a vital part of the software development and modeling processes. Such recognition by upper management must be translated into a commitment through policies that set quality goals, establish QA functions, and authorize necessary resources in terms of people, funding, and equipment to perform the tasks (Bryant and Wilburn 1987).

The QA organization should have a charter with each element of the organization defined and its responsibility outlined. The persons responsible for QA should be independent from those responsible for software development or model application. The QA organization must not be subordinate in any way to product development or delivery (Bryant and Wilburn 1987.)

Competent staffing is the key to a successful QA program. QA staff must have the respect of the project staff with which they work. They must understand how the work whose quality they are assuring is actually accomplished. Implementation of a successful QA program requires that all individuals involved understand what QA means, why it is being done, how they will benefit, what is expected of them, what are the responsibilities for each individual, and that good QA will help rather than hinder the modeling process (Bryant and Wilburn 1987). They should be convinced of the usefulness of QA and the importance given to it by management.

Closely related to and to a large extent crucial to the success of QA modeling are the capabilities of the modeling team. A good modeling team is multidisciplinary, includes highly trained and widely experienced senior staff, has effective internal communication, is managed by persons who have overview of the different disciplines involved in the project and who are able to translate management's questions into technical project objectives, and modeling results into advice to management. If such a team is well-managed QA forms an integral part of all its activities.

7. MANAGEMENT ISSUES IN GROUNDWATER MODELING

MANAGEMENT CONCERNS

Models have become widely accepted and quite useful as tools for drawing scientific conclusions and making technical decisions. However, models have not yet achieved great acceptance in the formulation of public policy. There are several reasons for the failure of policy makers to utilize models (OTA 1982, van der Heijde et al. 1985a). Individuals at higher levels of decision-making where policies are formulated often have less familiarity with models than the operation managers who use them for engineering decisions. Furthermore, policy decisions are increasingly contested in court. Evidence requirements in the litigation process are often difficult to meet, restricting management from incorporating modeling in their decision making. Opposing parties in a court of law frequently arrive at significantly different conclusions, sometimes based on the same model, thus contributing to management's reluctance to rely on models.

Management's lack of confidence in modeling probably reflects their experience with unsuccessful model application. Failures have been attributed to (1) use of insufficient or incorrect data; (2) incorrect use of available data; (3) inadequate conceptualization of the physical system such as flow in fractured bedrock; (4) use of invalid boundary conditions; (5) selection of an inadequate computer code; (6) incorrect interpretation of the computational results; and (7) providing answers to imprecise or wrongly posed management problems (OTA 1982, van der Heijde et al. 1985a, van der Heijde and Park 1986).

In some cases, insufficient scientific foundation with respect to basic processes and methodological principles has contributed to management's disappointment in model's predictive capabilities.

Groundwater managers have varied interests in model development, selection, and use, and in training modelers. In discussions with staff of one of the regulatory agencies, the U.S. EPA, the following major issues surfaced (van der Heijde and Park 1986):

- Limited knowledge of model availability
- The need for assistance in selecting and using adequate models for a specific site or specific use
- Guidance in establishing model reliability and interpretation of simulation results
- Improved interaction and communication with other professionals
- Training in basic processes (geology, hydrology, fate and transport, etc.) for the project managers in regulatory agencies as well as modeling training for the agencies' technical experts.
- Hiring and retaining technical staff who have received special training in modeling

- Need for ground-water modeling policies consistent with those in other areas of modeling.

Because of the deadlines and workload, project managers, who are often untrained in groundwater modeling, have no time to keep abreast of developments in modeling and, therefore, are often not qualified to introduce modeling into the project or to evaluate modeling done by contractors. Model application and interpretation of results is very subjective and may be the core of an expert's testimony in court. The expert's interpretation of results represents the culmination of months of technical work. Staff in regulatory agencies must be capable of providing the expert with both policy and technical oversight, e.g., in the quality assurance of the project. If this oversight is lacking, the expert's work may be misdirected or poor in quality. That this is a significant problem is illustrated by the modeling deficiencies frequently displayed in reported studies (van der Heijde and Park 1986).

A broad, multidisciplinary team is viewed as mandatory for adequate modeling of complex problems such as transport of hazardous waste. There is a tendency to underestimate staffing needs; and, even with breadth, staff tends to be spread too thin among projects.

High turnover in project managers, together with the inability to review the degree of success or failure in earlier projects, leaves little institutional memory for learning from previous studies. This leads to serious problems in the case of groundwater pollution studies, where the modeler or someone familiar with the application (e.g., the modeler's supervisor) often is required to serve as an expert witness. In addition to the familiarity with the study such a person needs to ensure the quality of the presentation to management of modeling results, and to the judge in the courtroom, an important aspect of the ultimate success of this kind of modeling.

Postmortem analyses of selected cases, with all staff informed, should be encouraged, so that the lessons learned can be communicated and applied to current and future site investigations. The results of such analysis should be made widely available.

The management issues involved are set forth in the final report of a study group for the EPA Office of Environmental Processes and Effects Research. The report examines issues related to that Agency's use of groundwater models and associated constraints (van der Heijde and Park 1986). According to the report, these issues can be divided into three groups: (1) the computer model being used, (2) application (conceptualization, data selection, and simulation), and (3) use of computational results in decision making. Issues of the first group include the assessment of the validity of computer codes. Prominent issues of the second group are criteria for selection of appropriate models for specific applications and review procedures for establishing model application, adequacy, and validity. The third group of issues relates only in part to modeling, as decision making is often based extensively on nontechnical considerations. A major limitation in addressing these issues is the scarcity of trained staff at all levels of management and technical services, both in government agencies and in private industry. To resolve many of the problems identified, the study group recommended that the

Agency adopt rigorous, well defined quality assurance procedures and establish extensive technology transfer and training programs.

Review of the important issues of the late 1970s and mid-1980s shows that despite many efforts to make improvements a significant number of problems still exist today (Bachmat et al. 1980, van der Heijde et al. 1985).

Major issues still of concern include inadequacies in models (formulation, testing, documentation), inadequacies in modeling (application, review), in communication between managers and technical personnel, and in training of model users and education of managers.

To further explore these issues, the Water Science and Technology Board recently established the Committee on Ground Water Modeling Assessment to examine the current state of knowledge concerning groundwater models and the role of contaminant models in the regulatory community (WSTB 1988). The 18-month study will address issues such as (1) the representation of physical, chemical, and biological processes in models of groundwater quality; (2) model formulation as related to observation of real groundwater systems; (3) model application procedures; (4) scientific, engineering, and policy trends influencing the future of modeling; (5) the role of models in decision making; and (6) the formulation of modeling guidelines and recommendations.

TECHNOLOGY TRANSFER AND TRAINING

As modeling for groundwater protection has become a rapidly growing area of technology and research, a vast body of information on technological and scientific advances is becoming increasingly available for groundwater management. Furthermore, the revolutionary advancement in computer software and hardware and the marked reduction in its cost has stimulated rapid adoption of groundwater modeling among groundwater professionals. The goal of technology transfer is to improve the systematic dissemination of information on groundwater modeling through communication and education. In its broadest sense, technology transfer includes development of application-oriented methods and models, the distribution of modeling codes and documentation, and training and assistance in model use (van der Heijde 1987b).

In 1982 the Office of Technology Assessment of the U.S. Congress (OTA) published a report on the use of models for water resources management, planning, and policy. Many of OTA's conclusions and recommendations on technology transfer and training apply to groundwater modeling today. The following OTA findings still apply:

- Levels of communication between decision makers and modelers are low, and little coordination of model development, dissemination, or use occurs within individual federal agencies.

- Developing and using models is a complex undertaking, requiring personnel with highly developed technical capabilities, as well as adequate budgetary support for computer facilities, collecting and processing data, and such support services as user assistance.

In general, technology transfer means dissemination of information on technological advances through communication and education. When applied to ground-water modeling, technology transfer includes dissemination of information about the role of modeling in water resource management, model theory, the process and management of modeling, availability and applicability of model software, information on quality assurance, model selection, and model testing and verification. It also pertains to the distribution of computer codes and documentation, and includes assistance in transferral, implementation, and use of codes.

The OTA report considers specific education and training of model developers, users, and managers in aspects of water resources modeling, as a critical component of technology transfer. Other technology transfer mechanisms include the distribution of published, printed, or electronically stored materials, such as reports, newsletters, papers, computer codes, data files, and other communications, and discussions and information exchanges in meetings, workshops, and conferences.

Effective communication forms the basis of technology transfer. Communication is often hampered because of insufficient communication channels, incompatible language or jargon, existence of different concepts, and administrative impediments.

Despite recent examples of successful modeling use in developing groundwater protection policies in the United States and abroad, managers still do not rely widely on modeling for decision making. One of the major obstacles is the inability of modelers and program managers to communicate effectively. An ill-posed problem yields answers to the wrong questions. Sometimes, this is the result of managers and modelers speaking different jargon.

On another level of communication, managers should appreciate how difficult it is to explain the results of complicated models to nontechnical audiences such as in public meetings and courts of law. Audio-visual aids are one useful means of overcoming these limitations in communication.

Training in Groundwater Modeling

Groundwater and groundwater modeling expertise often is disjunct within the groundwater community. Many inconsistencies in groundwater modeling have resulted.

The EPA Study Group (van der Heijde and Park 1986) concluded that among the modeling issues addressed during its meetings, improving the expertise of technical personnel deserves a high priority. Because it is expected that model use will increase in the future, the development of expertise on various levels of decision-making and technical assistance, by whatever means, appears to be a major priority.

A major impediment to meeting modeling needs is the inadequacy of current levels of model-related training and information exchange. If models are to be used effectively in water resources analysis, training in basic concepts of modeling and in proper interpretation of model results must be offered to decision makers at all levels of water resources management and environmental protection. Further, there is a need for specific training in the use of

individual models, and a need for continuingly informing and educating users and managers in research developments, new regulations and policies, and field experience.

The return on investments made in applying mathematical models to groundwater problems depends a great deal on the training and experience of the technical support staff involved in their use. Managers should be aware that specialized training and experience are necessary to develop and apply mathematical models, and that relatively few technical support staff can be expected to have such skills. This is due in part to the need for familiarity with a number of scientific disciplines, so that the model may be structured to faithfully simulate real-world problems. Managers should have some working knowledge of the sciences involved so that they might put appropriate questions to specialists. In practice this means that groundwater modelers, technical staff, and their supervisors should become involved in continuing education efforts, and managers should expect and encourage this. They should be sensitive to the financial and time requirements necessary for adequate training. (One does not become a competent modeler in a course of a week; that takes years and is a combination of training and experience.)

Mission-oriented organizations such as the USGS traditionally have given high priority to training and expertise. In regulatory agencies most technical and managerial personnel do not need to become modeling "experts," but should have sufficient training to be knowledgeable users or at least competent judges of the appropriateness of models used by third parties.

Information Exchange on Groundwater Modeling

There is an urgent need for expanding existing and developing new mechanisms to disseminate and exchange technical information. Two different approaches exist to information exchange: (1) the receiver actively seeks the required information or technology; (2) the receiver has a passive role insofar as supervisors or internal or external specialists bring the information or technology to the potential user.

When particular models are applied at particular sites, the experience needs to be institutionalized. A central clearinghouse should be created for keeping records on models used in a regulatory framework. The clearinghouse should have readily available information on: (1) where and under what conditions the models have been used; (2) what results were provided in terms of usefulness to management; and (3) what administrative, technical, and legal problems were encountered. This information should include contact persons, site descriptions, model modifications, and details on QA procedures.

A major impediment to meeting modeling needs is the inadequacy of model-related training and information exchange. Despite many efforts to resolve this obstacle, information from research projects often is not disseminated effectively to potential users. Recent legislation has demonstrated the renewed attention given to this problem (Section 209 of the Superfund Amendments and Reauthorization Act [SARA] of 1987).

PROPRIETARY CODES VERSUS PUBLIC DOMAIN CODES AND OTHER ACCEPTANCE CRITERIA

Is the use of proprietary codes in solving groundwater problems for or by government agencies acceptable, or should they be banned in favor of publicly accessible codes? Deciding this policy issue has become imperative in recent years, as an increasing number of modeling-based analyses performed by consultants or regulatory agencies in regulatory compliance cases are contested in the courtroom, and envrionmental decision-making processes in general are subject to increasing public scrutiny.

A proprietary code consists of computer software that is sold, leased, or used on a royalty basis, which generally conditions its use and limits its distribution. Some proprietary codes are publicly accessible, but restricted in transfer and use. According to this definition, proprietary codes used for solving groundwater problems could include: (1) groundwater simulation codes, (2) databases, (3) statistical packages, and (4) graphical packages. Public domain codes consist of software and documentation that can be used, copied, transferred, distributed, modified, or sold without any legal restrictions such as violation of copyrights.

There are various reasons why the use of proprietary codes is regarded problematic by the government (van der Heijde and Park 1986): lack of peer review and validation; problems with intercomparison and reproducability of results; administrative complications; and lack of access to software and theoretical basis. On the other hand, owners of proprietary code rights often promote the use of these codes for commercial, scientific, and other reasons.

Banning the Use of Proprietary Codes

Some agencies or their individual offices prefer the use of public codes if litigation is anticipated, assuming such code is available, even if the code is less efficient than an alternative proprietary code. Banning of proprietary codes is expected to eliminate some of the problems encountered in court cases. One of these problems is related to the notion that the code itself and its theoretical foundation might become contested. Unrestricted access to the computer code and documentation is considered crucial in such cases. However, if adequate model selection guidelines existed, including requirements for code review, validation, and documentation, and were applied consistently, such problems might be less significant.

Another issue is the inaccessibility of some proprietary codes and documentation. For example, EPA regulations (40 CFR 124.11 and 124.12) provide a mechanism for formal public hearings during the RCRA permit process. All aspects of EPA's decision making, including the use of groundwater models, are subject to public scrutiny. EPA use of models not accessible to the public may complicate the proceedings and result in EPA having to duplicate the modeling effort with a publicly accessible model. EPA's continued use of non-publicly accessible models increases the likelihood of Federal Open Information Act litigation. EPA policy restricting the use of nonpublicly accessible models may reduce this likelihood.

Furthermore, regulatory staff often does not have enough time and expertise to evaluate models or to go through a proper model selection process without support from model experts. However, this support can be provided

indirectly by establishing a list of reviewed and validated models and through various forms of guidance such as reports, and by expert systems. In such a certification process, public agencies tend to focus on public domain software.

Not all proprietary codes are publicly inaccessible. The private sector may control the use and dissemination of its computer models through copyright protection, patent protection, trade secret protection, or through a contractual or license agreement. Most of the issues discussed above result from attempts by some companies to maintain tight controls over their models through trade secret protection. The rationale is that a given model contains some formulation that makes it superior to those generally available, and that this formulation gives the company an advantage over its competitors. Exercising control through copyright protection and contractual agreements might be more difficult to enforce than trade secret protection. However, they allow for greater and quicker acceptance of the model by the technical community.

Continuing the Use of Proprietary Codes

Several reasons have been brought forward for the continued use of proprietary groundwater simulation codes:

- Use of proprietary codes encourages code development for solving new problems. If proprietary codes are banned, this incentive will be removed, greatly inhibiting future code development in the private sector. Because it is difficult for private companies to obtain funding for code development, the main justification for investing corporate funds in code development is the anticipation that some development costs will be recovered through code sales or value-added use. Capital gain is a major incentive for code development.

- Use of proprietary codes encourages private companies to enhance codes originally developed in the public domain. Many research-oriented codes developed in universities have been generalized, made user-friendly, and have been documented more fully by enterprising private developers. If the profit incentive is removed, further development and enhancement of public domain codes for applied purposes will be discouraged.

- Proprietary codes provide solutions to some problems that publicly available codes cannot solve. In some cases—for example, complex three-dimensional transport problems—publicly available codes are not adequate. Banning proprietary codes would eliminate the use of some of the more sophisticated codes. An alternative is to bring such a code into the public domain through outright purchase, and installing a service and support agreement with the code developers.

- Proprietary codes are often subject to rigorous internal QA. This is not always the case with public domain codes. If a code has problems (bugs), it will develop a bad reputation and will not sell, or will compromise the reputation of the company; a company is not likely to profit by selling inferior codes. In practice, however, many distributors of proprietary groundwater modeling software are relatively

small companies, some of which do not apply QA to model development and documentation. A model review and validation policy or procedural guidance should cull out the inferior models.

- User support might be available for proprietary codes. Once a proprietary code has been sold, it is in the interest of the seller to help the user apply the code in the best possible manner. Again, this does not always accur, as the smaller groundwater modeling software distributors often have limited resources for support and maintenance of their software. Often, consistent user support is not available for public domain codes.

- The use of proprietary databases, statistical packages, and graphical packages is rather widely accepted; the current regulatory questions focus specifically on the use of groundwater simulation codes. Policies applied to groundwater modeling software should be consistent with those established for other software.

It is necessary to establish consistent policies concerning selection and use of well tested and validated groundwater models. Such a policy should address the issues of model acceptance and use of proprietary codes and should be consistent with policies regarding surface water and air models. With respect to proprietary codes opinions vary from outright banning to ensuring a proper place for them in public policy (van der Heijde and Park 1986). In general, the following elements for such a policy regarding model acceptance are considered important:

- Establish a formal mechanism to review and validate models and define model acceptance criteria. This approach should be restricted to publicly available, noncopyrighted codes.

- Regulatory agencies should identify proprietary codes that it regards important to their mission; such codes should be brought into the public domain, after passing a review and validation process.

- A special list should be compiled of those proprietary codes that have passed a comparable review and validation process.

- Wherever possible the regulatory agency should advocate the use of publicly accessible groundwater modeling software.

The EPA Study Group (van der Heijde and Park 1986) recommended that a general framework of nondiscriminatory criteria should be established to apply to both public domain and proprietary codes. These criteria should include:

- Publication and peer review of the conceptual and mathematical framework

- Full documentation and visibility of the assumptions

- Testing of the code according to prescribed Agency methods; this should include verification (checking the accuracy of the computational algorithms used to solve the governing equations), and validation (checking the ability of the theoretical foundation of the code to describe the actual system behavior)

- Trade secrets (unique algorithms that are not described) should not be permitted if they might affect the outcome of the simulations; proprietary codes are already protected by the copyright law.

In case an agency policy includes acceptance of proprietary codes, provisions should be made regarding distribution of program copies of licensed software and documentation for purposes of regulatory compliance, as well as provisions for reasonable use by third parties (at reasonable cost) of code documentation and an executable version of the program code, or, at a minimum, access to the use of the code. Unreasonable cost to a group, such as a public interest group, could violate the provisions of the Freedom of Information Act.

For proprietary codes, an agency might also require from a contractor proof of copyright, ownership, or license to perform, display, and use the code. In case the agency intends to use the software internally, a license should be obtained to perform, display, use, and reproduce the code and related documentation in all parts of that agency.

In standardizing model selection, three major approaches are employed in characterizing the validation of numerical models. In one, the model is tested according to established procedures; when accepted, the model is prescribed in regulations for use in cases covered by those regulations. This approach does not leave much flexibility for incorporating the advances of recent research and technological development. The second approach includes the establishment of a list of groundwater simulation codes as "standard" codes for various generic and site-specific management puposes. To be listed, a code should pass a widely accepted review and test procedure. However, establishing "standard models" will not prevent discussion of the appropriateness of a selected model for analysis of a new policy or of its use in a particular decision-making process.

The question is, should standard models be established for an agency, such as EPA, or should criteria or guidelines be developed by which analysts can evaluate use of models. In considering this issue, questions have been raised such as:

- Are there legal liabilities for setting up certain models as acceptable? (For instance, if EPA certifies a model for a particular use, can the Agency no longer criticize an industry's selection of that model for other identical problems, or for that matter, even for solving non-identical problems?)

- Does certification squelch the development of new, better models?

- What balance should there be between using the newer, faster models and using mature models already subjected to peer review?

Another approach is to prescribe a review-and-test methodology in the regulations and require the model development team to show that the model code satisfies the requirements. This approach leaves room to update the codes as long as each version is adequately reviewed and tested. An example of this last approach is the quality assurance program for models and computer codes of the U.S. Nuclear Regulatory Commission (Silling 1983).

8. CURRENT LIMITATIONS OF MODELING; RECOMMENDATIONS FOR IMPROVEMENT

This report has focused on the principles of groundwater modeling and the status of modeling related software.

During the present decade a rapidly increasing number of sophisticated simulation models have become available for the evaluation of groundwater problems. These models are based on mathematical descriptions of the physical, chemical, and biological processes that take place in a complex hydrogeological environment. The extensive need for these models in assessing current and potential water management problems has resulted in two groups of modelers: (1) researchers who propose a conceptual representation of a groundwater system of interest and who generate computer codes to verify the mathematical descriptions derived from the modeled system and to evaluate the behavior of such a modeled system, and (2) model users who apply models routinely to actual groundwater management problems.

Accurate modeling of groundwater systems, especially where pollution is present, is limited by some fundamental problems. In the first place, not all processes involved are well understood and adequately described mathematically (Bear 1988). This is especially true for chemical and biological processes. For the most complex mechanisms, such as described by systems of coupled, highly non-linear equations, available numerical techniques are not always adequate (Pinder 1988). Finally, in most cases, lack of quantity or quality of data restricts model utility (Bear 1988, Konikow 1988).

Although major advances have been made in predicting the behavior of individual contaminants, studies of the interactions among contaminants are still in their infancy. Among others, these studies have focused on the ability of certain solvents to increase dramatically the mobility of ordinarily slow-moving pesticides, of polynuclear aromatic hydrocarbons, and of other substances.

Other areas where substantial progress is needed lie in understanding the immiscible flow and transport considerations so crucial to solving the problems of leaking underground storage tanks, and the manner in which contaminant transport in fractured rocks differs from transport through porous sediment.

Improvements are required, concurrently, in several other major areas. Data acquisition methods and interpretive models are needed that can examine to an unprecedented degree the physical, chemical, and biological processes controlling the transport and fate of groundwater contaminants. Unfortunately, few of the constants and coefficients needed to incorporate chemical and biological processes into contaminant transport evaluations are available.

THE ROLE OF DATA

Modeling provides a framework to order and interpret data within the decision-making process. The effectiveness of any model is dependent on the accuracy of the data acquired. In many applications, the lack of data inflicts a severe constraint upon obtaining useful model results. Therefore, the use of computer models in groundwater resource development and protection

will continue to be limited mainly by the time and costs incurred in collecting sufficient and accurate hydrologic and geologic data for proper description of groundwater systems and their functional characteristics. This does not mean, however, that some indication of the relative contribution of various processes to a groundwater system's total response cannot be estimated; much of the existing information can be used in a semiquantitative manner (i.e., sensitivity analyses and "worst-case" scenarios).

Efforts to collect field data and to estimate natural-process parameters must be expanded and improved so that model applications will be more physically based and thereby capable of more accurate predictions. For example, so few data are available concerning the exact location, volume, composition, and timing of chemical releases at existing sites that it is very difficult for modelers to determine the appropriate configuration of what is referred to as the "source term" in modeling. One prevailing misconception in this regard is the idea that additional chemical sampling of monitoring wells can provide definitive clues to the missing historical data; this is true only superficially. Although indication of the source term can be obtained from the patterns of chemical movement, there is no guarantee that causal relationships can be discovered or that the patterns will remain constant.

A common misconception is that all field methods and tools necessary for obtaining data to run the models are available, if not in optimal form, at least in a useful form. In fact, however, direct measurements are unreliable or cannot be obtained for a number of parameters such as groundwater flow velocity and direction, rates of sorption and desorption (retardation) of organic chemicals, and the potential for biotransformation. This misconception parallels the mistaken idea that all necessary theories have been worked out and that further refinements are needed only to provide precision and accuracy.

The integration of geologic, hydrologic, chemical, and biological processes into usable subsurface flow and transport models is possible only if the data and concepts invoked are sound. The data must be representative as well as accurate and precise. The degree to which the data are representative is relative to the scale of the problem and the concepts guiding data collection and interpretative efforts. Careful definition of these concepts is crucial; special attention should be given to the spatial and temporal variations involved.

The use of newly developed theories to help solve field problems is often a frustrating exercise. Most theoretical advances call for some data not yet practically obtainable (e.g., chemical interaction coefficients and relative permeabilities of immiscible solvents and water). In addition, the incorporation of theoretical relationships into mathematical models typically is made possible by invoking certain assumptions and simplifications that alter the intended relationship. Therefore, theoretical advances in modeling groundwater problems must be accompanied by improvements in data collection and mathematical representation efforts.

Large numerical models are particularly data-hungry. Incorporating new geochemical, hydrological, and biochemical processes often stretches existing data collection capabilities beyond a practical limit. In many cases generic data are required, obtained from laboratory batch experiments or controlled

field experiments. Centralized management of such datasets and efficient dataset referral services are of great importance to the groundwater modeling community.

MANAGEMENT ISSUES IN MODELING

Although the precise formulation of a management problem can be quite thorny, it is prerequisite to the solution. The manner in which a problem is defined bears heavily on how the professional approaches a solution. Improved problem definition is likely to result from more interactive participation of managers and technical personnel in model design and application, both in a project's initial stage, as is usually the case, and during the modeling effort itself. Code output is often a barrier to more effective utilization of the code. Program managers and decision makers need to have model results presented in a way that is both meaningful and compatible with decisions that must be made. The uncertainties contained in various decision alternatives are especially important to assess.

The economic consequences of model predictions and the potential liabilities incurred by their use have brought quality guarantees and code credibility to the forefront as major issues in groundwater modeling. Hence, quality assurance (QA) needs to be defined and implemented for both model development and model application. There is a significant difference between these two: the first is designed to result in a generally reliable code, and the second to obtain reliable predictions for existing field conditions under prevailing management constraints. Both require stringent QA procedures. To further increase the applicability of the models, good documentation and user-friendliness of the computer coding involved should receive close attention.

Parallel with, and to a significant extent responsible for the rapid increase in groundwater modeling capabilities, is the technological advance in computer hardware and software. This is especially noticeable in the integrated approach to computer-based decision-support systems in groundwater management. In these hardware-software systems, data acquisition and control is combined with analytical, optimization, and presentational techniques, resulting in an efficient management tool. The recent introduction of artificial-intelligence-based expert system technology promises further advances in the utility and sophistication of decision-support technology.

Managers should require computer-processible data; a protocol for database management systems, improved data-processing techniques, and standardized formats for I/O (input-output) should be adopted. This will significantly improve the efficiency of modeling-based data analyses needed for the resolution of many groundwater issues.

RESEARCH NEEDED

The earlier-quoted EPA Study Group has identified a variety of new models and modeling approaches as important to groundwater protection (van der Heijde and Park 1986):

- Simulation of flow and transport in multimedia (e.g., coupled models for surface water/ground-water interaction)

- Representation of stochastic processes in predictive modeling, and improving the applicability of geostatistical models
- Improved modeling of hydrochemical speciation
- Simulation of flow and transport in fractured and dual-porosity media, including diffusion in dead-end pores
- Simulation of flow and transport in soils containing macropores
- Determination of effects of concentration-dependent density on groundwater flow and pollutant transport
- Determination of effects of alteration of geologic media on hydrological and chemical characteristics (e.g., dehydration of clay when attacked by solvents, change in sorptive capacity of material when heated)
- Representation of the three-dimensional effects of partially penetrating wells on water table aquifers
- Development of models for management of groundwater contamination plumes
- Development of expert systems (artificial intelligence) for such tasks as selecting appropriate submodels or subroutines for specific problems
- Application of parameter identification models to be used with site studies
- Further development of pre- and postsimulation data processors
- Continued development of risk assessment and management models
- Modeling of volatilization, multiphase flow, and immiscible flow
- Incorporation of economic factors to improve estimation of cleanup costs
- Development of generic and site-specific parameter databases.

Fundamental research supporting groundwater modeling is considered necessary in such areas as:

- Transient behavior of process parameters (e.g., retardation, hydraulic conductivity)
- Desorption for nonhydrophobic chemicals
- Multicomponent transport and chemical interaction
- Enhanced transport mechanisms (e.g., piggy-backing on more mobile chemicals)

- Transport of silt with sorbed chemicals in aquifers

- Improved numerical accuracy, stability, and efficiency.

Modeling the transport and fate of chemicals in groundwater is a major subject of several research programs (DOE 1985, EPA 1987). These programs focus on immiscible flow associated with organic and oil-like liquids (DOE 1986, EPA 1987). Other topics currently being studied include simulation of flow and transport in fractured and dual-porosity media, representation of stochastic processes in predictive modeling, multimedia risk assessment, incorporation of volatilization in multiphase transport models, and simulation of density-dependent flow.

CLOSURE

Current and near-future research on geochemical, hydrological, and biophysical mechanisms, including large- intermediate- (e.g., artificial aquifers), and field-scale experiments, will probably lead to increasingly sophisticated mathematical tools for analysis of a variety of groundwater problems, taking into consideration the stochastic nature of many of the processes involved. Such problems will not be restricted to water supply and water pollution issues, but may include other aspects of subsurface use, as for geothermal energy generation, subsurface energy storage, in-situ ore processing, and foundation engineering. The complexity of the resulting models will require a significant increase in computer resources, validation opportunities, and user expertise. Datasets generated in field-scale experiments will be particularly useful for retrospective model validation. Along with the growing complexity of groundwater models and methodologies, user expertise must expand through education and training.

In many respects, modeling will be made easier and "flashier" by the rapidly evolving computer hardware and software technologies. The mechanics of entering data, running simulations, and creating high-quality graphics will become less time-consuming and less complex. Such a reduction of time and effort may lead to the dangerous assumption that modeling seems to be simple. In fact, however, modeling will become more and more challenging as groundwater specialists deal with increasingly complex natural systems and management problems, and as the gap widens between our capabilities to characterize the real world by measuring and simulating simplified images of real-world systems. Ultimately, it should be the multidisciplinary team representing the combined knowledge of several fields of expertise that passes judgment on a management issue, and not the modeler and certainly not "the model." A model is not more than a tool, albeit a complex one, and a model user should be more than someone who knows how to handle the tool. As the role of models in decision making increases, the consequences of incorrect model use become more critical. To draw on a common metaphor: it seems easy to hit a nail with a hammer, but no one wants to be the person who misses the nail while someone else holds it!

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APPENDIXES A–H

The following appendixes contain descriptive listings of selected models from the IGWMC MARS database. The IGWMC model information databases are accessible through the IGWMC offices in Indianapolis, Indiana, and Delft, The Netherlands. The models listed are considered by the authors to be relevant, available (as defined in the section on model selection of Chapter 4), and current. Model categories are saturated groundwater flow (A1, A2), variable saturated flow (B1, B2), solute transport (C1, C2), heat transport (D1, D2), hydrogeochemical speciation (E1, E2), flow and transport in fractured rock (F1, F2), and multiphase flow (G1, G2). Two tables are provided for each category. The first table (e.g., A1) identifies the models, provides contacts, and describes the capabilities of each model. The second table (e.g., A2) for a given category provides additional information for evaluating a model's usefulness and reliability.

As discussed in the section on model selection in Chapter 4, an important aspect of a model's use in ground-water management is its efficiency, which is determined by the human and computer resources required for its proper operation. A model's efficiency can be described by its usability, availability, modifiability, portability, and economy of computer use. Another important issue is the model's reliability. In the appendixes, usability and reliability are qualified by the following descriptors.

USABILITY

Pre- and Postprocessors

The presence of pre- and postprocessors is rated as: not present [none, N], dedicated [model-dependent, D], generic [can be used for a class of models, might include separate reformatter for specific models or display software, G], used for interactive runs [I], or status unknown [U].

Documentation

As part of assessing the adequacy of the documentation, the presence of an adequate description of user's instructions and example datasets is indicated by yes [Y] or no [N]. Models having no published description of their theoretical basis are not listed in these appendices.

Support

Software support and maintenance is rated as: none [N], limited with respect to level of support [L], unlimited [Y], and unknown [U].

Hardware Dependency

In this report a model's hardware and/or software dependency is indicated as present [Y] or not [N]. Hardware dependency may be due to the size of the source code, the way it has been designed and compiled, the use of specific peripherals, and graphics calls in the program. In addition, programs may be software-dependent, requiring specific program purchases to reside on the user's computer (e.g., graphics or mathematical routines).

RELIABILITY

Review

This report identifies peer-review of theory and coding. For each category the rating is: peer-reviewed [Y], not peer-reviewed [N], and unknown [U]. A model is considered to be peer-reviewed if theory and code has been subject to a formal review process such as established by certain agencies (eg., U.S. EPA, U.S. Geological Survey). In addition, a model's theory is considered to be peer-reviewed if it has been published in a peer-reviewed journal (e.g., ***Water Resources Research***).

Verification

A model's verification status is rated as extensive [Y], not verified [N], or unknown [U]. Models verified only with respect to segments of their coding or for only a part of the tasks for which they were designed are rated to have undergone partial or limited verification [L].

Field Testing

In this report, model field testing, the application of models to site-specific conditions for which extensive datasets are available (see Chapter 3), is rated as extensive [y], partial or limited [L], not validated [N], or unknown [U].

Extent of Model Use

This report evaluates the extent of a model's use in four classes: many [M, >10], few [1–10], none [N], and unknown [U].

Appendix H is a list of principle references for the models listed in A–G. Note that model reference numbers are listed under the author entry in tables A1–G1. Similarly, each reference in Appendix H includes the appendix number and IGWMC key number of the model to which that reference applies.

For additional information contact IGWMC-Indianapolis, Holcomb Research Institute, Butler University, 4600 Sunset Avenue, Indianapolis, Indiana 46208, or IGWMC-Delft, TNO-DGV Institute of Applied Geoscience, P.O. Box 285, 2600 AG, Delft, The Netherlands.

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	S.P. Neuman P.A. Witherspoon Ref: 116	Department of Hydrology and Water Resources University of Arizona Tucson, AZ 85721	FREESURF I (1979)	A finite-element model to simulate two-dimensional vertical or axisymmetric, steady-state flow in an anisotropic, heterogeneous, confined or water-table aquifer.		0020
2.	S.P. Neuman P.A. Witherspoon Ref: 117	Department of Hydrology and Water Resources University of Arizona Tucson, AZ 85721	FREESURF II (1979)	A finite-element model to simulate two-dimensional vertical or axisymmetric, transient flow in anisotropic, heterogeneous porous media with free surfaces.		0022
3.	T.R. Narasimhan Ref: 112	National Energy Software Center (NESC) Argonne National Lab. 9700 South Cass Avenue Argonne, IL 60439	TERZAGI (1981)	An integrated-finite-difference approach to compute steady and non-steady pressure head distributions and one-dimensional compaction in saturated, heterogeneous, anisotropic porous media with complex geometry.	consolidation expansion leakage compaction	0121
4.	R.L. Cooley J. Peters Ref: 26	Hydrologic Engineering Center U.S. Army Corps of Engineers 609 Second Street Davis, CA 95616	ECPL 723-G2-L2440 (1981)	A finite-element solution for determining head distributions in confined, semi-confined, or unconfined, anisotropic, heterogeneous aquifer systems. The model can handle horizontal, cross-sectional, or axisymmetric configurations for steady-state flow.	leakage	0140
5.	R.L. Cooley J. Peters Ref: 26	Hydrologic Engineering Center U.S. Army Corps of Engineers 609 Second Street Davis, CA 95616	FINITE ELEMENT SOLUTION OF STEADY-STATE POTENTIAL FLOW PROBLEMS (1981)	A finite-element solution to simulate steady-state axisymmetric flow through a heterogeneous anisotropic, leaky aquifer.	capillary forces leakage	0141
6.	R.L. Cooley R.L. Naff Ref: 27	U.S. Geological Survey Water Resources Division Box 25046, MS 413 Federal Center Denver, CO 80225	NON-LINEAR REGRESSION GROUNDWATER FLOW MODEL (1985)	An interactive inverse groundwater flow model using non-linear regression and finite-element simulation. It estimates source/sinks, boundary fluxes and best fit hydraulic head distribution for steady-state, horizontal groundwater flow in an anisotropic, heterogeneous aquifer.	leakage delayed yield	0195

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
7.	H.J. Morel-Seytoux C. Rodriquez C. Daly T. Illangasekare G. Peters Ref: 111	Colorado State University Engineering Research Center Fort Collins, CO 80523	DELTA (1981)	A two-dimensional areal model to simulate transient groundwater flow in a confined or unconfined heterogeneous, isotropic aquifer connected with a river, using stream-aquifer response coefficients.	infiltration	0260
8.	T.A. Prickett C.G. Lonnquist Ref: 137	Consulting Water Resource Engineers 6 G.H. Baker Drive Urbana, IL 61801	PLASM (1971)	A finite-difference two-dimensional or quasi-three-dimensional, transient, saturated flow model for single layer or multi-layered confined, leaky confined, or water-table aquifer systems with optional evapotranspiration and recharge from streams.	evapotranspiration leakage	0322
9.	G.F. Pinder E.O. Frind Ref: 132	Department of Civil Engineering Princeton University Princeton, NJ 08540	ISOQUAD (1982)	Finite-element model to simulate three-dimensional groundwater flow in confined and unconfined aquifers.	leakage	0510
10.	G.F. Pinder C.I. Voss Ref: 135	U.S. Geological Survey Water Resources Division National Center, MS 431 Reston, VA 22092	AQUIFEM (1979)	A finite-element model to simulate transient, areal groundwater flow in an isotropic, heterogeneous, confined, leaky-confined or water table aquifer.	leakage infiltration	0514
11.	P.S. Huyakorn Ref: 81	Performance Assessment Department Office of Nuclear Waste Isolation Battelle Project Management Division 505 King Avenue Columbus, OH 43201	STAFAN 2 (1982)	A finite-element model for simulation of transient two-dimensional flow and stress in deformable fractured and unfractured porous media.	deformation compaction	0584
12.	T.R. Knowles Ref: 164	Texas Department of Water Resources P.O. Box 13087 Austin, TX 78758	GWSIM (1981)	A transient, two-dimensional, horizontal model for prediction of piezometric head in an anisotropic, single-layer aquifer.		0681
13.	C.R. Faust T. Chan B.S. Ramada B.M. Thompson Ref: 82	Performance Assessment Department Office of Nuclear Water Isolation Battelle Project Mgmt. Division 505 King Avenue Columbus, OH 43201	STFLO (1982)	A linear finite-element code for simulation of steady-state, two-dimensional (areal or vertical) plane or axisymmetric groundwater flow in anisotropic, heterogeneous, confined, leaky or water-table aquifers.	leakage	0694
14.	S.B. Pahwa B.S. Rama Rao Ref: 83	Performance Assessment Department Office of Nuclear Waste Isolation Battelle Project Mgmt. Division 505 King Avenue Columbus, OH 43201	NETFLO (1982)	To simulate steady-state three-dimensional flow in a heterogeneous medium by an equivalent network of series and parallel flow members.		0695

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
15.	T. Maddock III Ref: 165	Water Resources Development and Management Service Land and Water Development Organization Food and Agriculture Organization of U.N. Via Delle Terme de Caracella, 00100 Rome Italy	LEAKY AQUIFER SIMULATION (1982)	To calculate the response of an isotropic, heterogeneous, confined or leaky aquifer to pumping from one or more wells, based on horizontal two-dimensional, unsteady-state flow simulation.	leakage	0756
16.	P.C. Trescott S.P. Larson Ref: 171	U.S. Geological Survey Branch of Groundwater MS 411, National Center Reston, VA 22092	USGS-3D-FLOW (1982)	A finite-difference model to simulate transient, three-dimensional and quasi-three-dimensional, saturated flow in anisotropic, heterogeneous groundwater systems.	evapotranspiration leakage	0770
17.	P.C. Trescott G.F. Pinder S.P. Larson Ref: 172	U.S. Geological Survey Branch of Groundwater MS 411, National Center Reston, VA 22092	USGS-2D-FLOW (1976)	A finite-difference model to simulate transient, two-dimensional horizontal or vertical flow in an anisotropic and heterogeneous, confined, leaky-confined or water-table aquifer.	leakage evapotranspiration	0771
18.	V. Guvanasen Ref: 65	Department of Civil and System Engineering James Cook University of North Queensland Queensland, 4811 Australia	I.D.P.N.G.M. (1979)	Finite-difference approach for the direct inverse problem of parameter identification in a confined or unconfined heterogeneous isotropic aquifer with transient two-dimensional horizontal groundwater flow.		0951
19.	K.R. Rushton L.M. Tomlinson Ref: 148	Department of Civil Engineering University of Birmingham P.O. Box 363 Birmingham, B15 2TT United Kingdom	AGU-1 (1979)	Finite-difference model for transient single layered two-dimensional horizontal groundwater flow.	leakage	1230
20.	M. Clouet D'Orval	Burgeap 70, Rue Mademoiselle 75015 Paris France	BURGEAP 7600 HYSO PACKAGE (1982)	A program package to simulate two-dimensional, horizontal/vertical, steady/transient, saturated flow in confined/unconfined, homogeneous/heterogeneous aquifer systems with multiple immiscible fluids, and connection with surface water.		1370
21.	M. Clouet D'Orval	Burgeap 70, Rue Mademoiselle 75015 Paris France	BURGEAP 7600 HYSO (TRABISA MODEL) (1981)	To simulate two-dimensional, horizontal, transient, saturated flow of two immiscible fluids of different densities, in unconfined, homogeneous/heterogeneous aquifers.		1371

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
22.	M. Clouet D'Orval	Burgeap 70, Rue Mademoiselle 75015 Paris France	BURGEAP 7600HYSO (TRABICO MODEL) (1981)	Simulation of two-dimensional, vertical transient flow in heterogeneous, confined or unconfined aquifers with representation of free surface to determine the hydraulic coefficients pertaining to the relation between a river and the aquifer.		1372
23.	A. Levassor	Centre D'Informatique Geologique Ecol Des Mines De Paris 35, Rue Saint-Honore 77305-Fontainbleau France	PLIN (1981)	Optimization of well field exploitation in single or multi-layered aquifer system using influence coefficients.		1470
24.	P. Prudhomme J.L. Henry F. Biesel	Laboratoire Central D'Hydraulique De France 10, Rue Eugene-Renault 94700 Maisons-Alfort France	BIDAT-HS2 (1981)	A finite-difference model for prediction of piezometric heads and flow in anisotropic, heterogeneous, confined, semi-confined, or unconfined aquifers.	leakage infiltration	1481
25.	P. Prudhomme J.L. Henry F. Biesel	Laboratoire Central D'Hydraulic De France 10, Rue Eugene-Renault 9700 Maisons-Alfort France	TRIGAT-HS1 OR AXYZ-HS5 (1981)	A finite-difference model for prediction of piezometric heads for unsteady three-dimensional flow in confined, semi-confined or unconfined, anisotropic, heterogeneous aquifers.	leakage	1482
26.	B. Boehm	Abteilung Wasserwirtschaft Rheinbraun Stuttgenweg 2 5000 Koln 41 Federal Republic of Germany	GW 1 (1981)	A transient, two-dimensional finite-difference groundwater model to simulate dewatering in isotropic, heterogeneous aquifers, using polygons.	dewatering	1531
27.	Y. Bachmat A. Dax	Hydrological Service of Israel P.O. Box 6381 Jerusalem, Israel	ITERATIVE ALGORITHM FOR SOLVING THE INVERSE PROBLEM IN A MULTICELL AQUIFER MODEL (1979)	This model solves the inverse problem in a two-dimensional water-table aquifer with varying pumping and replenishment.		1631
28.	D.A. Blank	Tahal Consulting Engineers Ltd. P.O. Box 11170 Tel Aviv, Israel	AQSIM (1981)	A two-dimensional finite-difference model to solve transient horizontal groundwater problems in isotropic, heterogeneous, confined or phreatic aquifers connected with a stream; optional simulation of salt-fresh water interface.	infiltration	1651

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
29.	H.M. Haitjema O.D.L. Strack	School of Public and Environmental Affairs 10th Street Indiana University Bloomington, IN 47405	SYLENS (1985)	An analytical solution for steady-state groundwater flow in regional double aquifer systems with local interconnections.	infiltration evapotrans-piration	1791
30.	T.N. Olsthoorn	Nansenlaen W. 9641 XW Pynacker The Netherlands	TOFEM-N (1985)	Multi-layer finite-element groundwater flow model.		1814
31.	C. van den Akker Ref: 175	National Institute for Water Supply P.O. Box 150 2260 AD Leidschendam The Netherlands	FLOP (1981)	A finite-difference model for calculation of pathlines in confined aquifers without storage and residence times of water particles.		1820
32.	C. van den Akker Ref: 175	National Institute for Water Supply P.O. Box 150 2260 AD Leidschendam The Netherlands	FLOP-2 (1981)	To generate pathlines for steady-state flow in a semi-confined, isotropic, homogeneous aquifer without storage and to calculate residence times for a number of water particles.		1821
33.	C. van den Akker Ref: 175	National Institute for Water Supply P.O. Box 150 2260 AD Leidschendam The Netherlands	FRONT (1981)	Calculation of pathlines for steady-state and transient flow in a confined, isotropic, heterogeneous aquifer and computation of residence times for a number of water particles.		1822
34.	P. van der Veer	Rijkswaterstaat Data Processing Division P.O. Box 5809 2280 HV Rijswijk (Z.H.) The Netherlands	MOTGRO (1981)	Prediction of groundwater head and stream function for two-dimensions using analytical function method; vertical, steady and unsteady, single or multi-fluid flow in homogeneous, anisotropic, confined or unconfined aquifers or arbitrary shapes.		1830
35.	A. Verruijt J.B.S. Gan Ref: 186	Department of Civil Engineering Delft Technical University Sterinweg 1 2628 CN Delft The Netherlands	SWIFT (1982)	A cross-sectional finite-element model for transient horizontal flow of salt and fresh water and analysis of upconing of an interface in a homogeneous aquifer.	buoyancy leakage	1852
36.	D.E. Evenson Ref: 47	CDM Water Resources Engineers 710 South Broadway Walnut Creek, CA 94596	PEP (1981)	To calibrate steady or unsteady, confined or water-table flow models for anisotropic heterogeneous aquifer systems automatically by non-linear programming techniques.	infiltration	1940

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
37.	K. Ueshita K. Sato Ref: 173	Department of Geotechnical Eng. Nagoya University Chikusa, Nagoya 464 Japan	CONSOL-1 (1981)	A non-steady-state finite-element model to simulate one-dimensional vertical groundwater flow and soil displacement in order to calculate the groundwater levels necessary for the prevention of land subsidence.	consolidation	2021
38.	H.J. Morel-Seytoux T. Illangasekare Ref: 79	Engineering Research Center, A315 Colorado State University Fort Collins, CO 80523	DELTIS-STREAM-AQUIFER DISCRETE KERNEL GENERATOR (1981)	A stream-aquifer discrete kernel generator for horizontal confined or unconfined, transient groundwater flow in isotropic, heterogeneous aquifers.		2060
39.	H.J. Morel-Seytoux C.J. Daly G. Peters Ref: 130	Engineering Research Center, A315 Colorado State University Fort Collins, CO 80523	DELPET-DISCRETE KERNEL GENERATOR (1977)	A discrete kernel generator for transient horizontal flow in an isotropic, heterogeneous, confined or unconfined aquifer to simulate drawdowns and return flows.	evapotranspiration	2061
40.	S.K. Gupta C.R. Cole F.W. Bond Ref: 61	Water and Land Resources Division Battelle Pacific NW Lab. P.O. Box 999 Richland, WA 99352	FE3DGW (1985)	Transient or steady-state, finite-element three-dimensional simulation of flow in a large multi-layered groundwater basin.	leakage delayed yield compaction infiltration	2072
41.	A.E. Reisenauer C.R. Cole Ref: 15	Water and Land Resources Division Battelle Pacific NW Lab P.O. Box 999 Richland, WA 99352	VTTSS3 (1979)	A finite-difference model to predict steady-state hydraulic head in unconfined or confined multi-layered aquifer systems and to generate streamlines and traveltimes.	leakage infiltration	2090
42.	A.E. Reisenauer C.R. Cole Ref: 15	Water and Land Resources Division Battelle Pacific NW Lab P.O. Box 999 Richland, WA 99352	VTTSS2 (1979)	A finite-difference model to predict steady-state hydraulic head in confined aquifers systems with up to five layers.	leakage infiltration	2091
43.	A.E. Reisenauer C.R. Cole Ref: 15	Water and Land Resources Division Battelle Pacific NW Lab P.O. Box 999 Richland, WA 99352	VTT (1979)	A finite-difference model to calculate transient hydraulic head distributions in confined or unconfined multi-layered aquifer systems, and to generate traveltimes.	leakage infiltration	2092
44.	J.W. Mercer C.R. Faust Ref: 109	Geotrans, Inc. 250 Exchange Pl. Suite A Herdon, VA 22070	SWSOR (1980)	A finite-difference model to simulate the areal, unsteady flow of saltwater and freshwater separated by an interface in anisotropic, heterogeneous porous media.	leakage infiltration	2140

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
45.	J.B. Weeks Ref: 18	U.S. Geological Survey Water Resources Division Box 25046, MS 412 Denver Federal Center Lakewood, CO 80225	QUASI THREE-DIMENSIONAL MULTIAQUIFER MODEL (1978)	A finite-difference model to simulate transient or steady-state groundwater flow in isotropic, heterogeneous multi-aquifer systems.	leakage	2510
46.	L.R. Townley J.L. Wilson A.S. Costa Ref: 168	Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics Room 48-211 Massachusetts Institute of Technology Cambridge, MA 02139	AQUIFEM-1 (1979)	A two-dimensional, finite-element model for transient, horizontal groundwater flow.	leakage	2630
47.	L.K. Kuiper Ref: 99	U.S. Geological Survey SW Tower, 3rd floor 211 East 7th Street Austin, TX 78701	VARIABLE DENSITY MODEL (1984)	Integrated-finite-difference model for the simulation of variable density groundwater flow in three dimensions.	evapotranspiration	2663
48.	R.H. Page Ref: 126	Water Resources Program Department of Civil Engineering Princeton University Princeton, NJ 08540	INTERFACE (1979)	To simulate transient flow of fresh and saline water as immiscible fluids separated by an interface in an isotropic, heterogeneous, water table aquifer using the finite-element method.		2720
49.	D.R. Posson G.A. Hearne J.V. Tracy P.F. Frenzel Ref: 136	U.S. Geological Survey P.O. Box 26659 Albuquerque, NM 87125	N.M.F.D 3D (1980)	A finite-difference model for simulation of unsteady two-dimensional horizontal groundwater flow in multi-layered heterogeneous anisotropic aquifer systems or unsteady three-dimensional saturated flow systems.	leakage	2740
50.	C.J. Daly Ref: 29	U.S. Army Corps of Engineers Cold Regions Research & Engineering Lab Hanover, NH 03755	CRREL (1984)	Analytical model to calculate and plot streamlines for flow in anisotropic, heterogeneous aquifers.		2791
51.	J. Boonstra Ref: 16	Intern'l Inst. for Land Reclamation and Improvement P.O. Box 45 Wageningen The Netherlands	S.G.M.P. (1981)	Uses integrated-finite-difference approach for simulation of steady-state or transient, two-dimensional, horizontal flow in a saturated, anisotropic, and heterogenous, confined, semiconfined or phreatic aquifer.	leakage	2800
52.	O. Berney Ref: 12	Land and Water Development Division Food and Agriculture Organization Via Delle Terme Di Caracalla 00100-Rome Italy	DISIFLAG (1980)	A finite-difference model for steady-state or transient simulation of two-dimensional, horizontal groundwater flow in a two-layered, isotropic, heterogeneous aquifer system.	leakage	2870

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
53.	H.N. Tyson Ref: 12	Water Resources Development and Management Service Land and Water Development Division Food and Agriculture Organization of the United Nations Via Delle Terme Di Caracalla, 00100 Rome, Italy	KRGW (1982)	A finite-difference model to simulate steady-state or transient, two-dimensional horizontal flow in a single confined or unconfined, or a two-layered, leaky, isotropic, heterogeneous aquifer system.	leakage	2930
54.	A.P.M. Broks D. Dijkstra J.W. Wesseling Ref: 19	Delft Hydraulics Lab P.O. Box 152 8300 AD Emmeloord The Netherlands	GROMULA (1981)	A user-oriented finite-element model to simulate steady-state or transient, two-dimensional groundwater flow in anisotropic, heterogeneous, multi-layered aquifer systems.	leakage	2980
55.	B.H. Gilding J.W. Wesseling Ref: 55	Delft Hydraulics Lab P.O. Box 152 8300 AD Emmeloord The Netherlands	GROMAGE (1982)	Finite-element solution for transient simulation of two-dimensional horizontal groundwater flow and drainage in anisotropic heterogeneous multi-layered aquifer systems.	evapotranspiration drainage	2981
56.	J. Noorishad P.A. Witherspoon	Earth Sciences Division Lawrence Berkeley Lab University of California Berkeley, CA 94720	ROCMAS-H (1976)	A finite-element model for two-dimensional simulation of transient groundwater flow in porous fractured rock.		3080
57.	J. Noorishad M.S. Ayatollahi P.A. Witherspoon Ref: 124	Earth Sciences Division Lawrence Berkeley Lab University of California Berkeley, CA 94720	ROCMAS-HM (1981)	A finite-element two-dimensional model for analysis of quasi-static coupled stress and fluid flow in porous fractured rock.	consolidation fracture deformation	3082
58.	G. Schmid Ref: 155	Ruhr-University Bochum Institute F. Konst. Ingenieubau AG IV D-4630 Bochum Federal Republic of Germany	SICK 100 (1981)	Simulation of vertical and horizontal steady and non-steady groundwater flow, using potential and stream function approach.	delayed yield	3110
59.	P.M. Cobb C.D. Mcelwee M.A. Butt Ref: 108	Kansas Geological Survey 1930 Avenue A, Campus W University of Kansas Lawrence, KS 66044	TSSLEAK (1982)	Automated analysis of pumping-test data for a leaky-artesian aquifer.	leakage	3160
60.	B. Sagar	Analytic and Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	AQUIFER (1982)	Analysis of steady and non-steady-state, two-dimensional areal or cross-sectional, radial flow in heterogeneous, anisotropic multi-aquifer systems.	leakage infiltration	3230

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
61.	B. Sagar Ref: 150	Analytic and Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	DEWATER (1982)	Uses integrated-finite-difference approach for two-dimensional, areal or cross-sectional, radial simulation of steady or unsteady flow in anisotropic and heterogeneous, confined or water table aquifers; predicts drawdown due to pumping during surface and subsurface mining and building construction operations.	dewatering	3231
62.	J.A. Liggett Ref: 103	School of Civil and Environmental Engineering Hollister Hall Cornell University Ithaca, NY 14853	GM5 (1982)	Uses boundary integral equation modified for steady-state simulation of three-dimensional saturated groundwater flow in an anisotropic, heterogeneous multi-aquifer system.	leakage	3240
63.	P.J.T. van Bakel Ref: 174	Institute for Land and Water Management Research P.O. Box 35 6700 AA Wageningen The Netherlands	FEMSAT (1981)	A finite-element model to simulate transient two-dimensional horizontal flow in a saturated heterogeneous, anisotropic multi-layered aquifer system.	leakage	3350
64.	G.T. Yeh C.W. Francis Ref: 196	Environmental Sciences Division Oak Ridge National Laboratory Oak Ridge, TN 37830	AQUIFLOW (1984)	A two-dimensional finite-element model to simulate transient flow in horizontal, anisotropic, heterogeneous aquifers under confined, leaky or unconfined conditions.	leakage	3372
65.	G.T. Yeh D.D. Huff Ref: 197	Environmental Sciences Division Oak Ridge National Lab Oak Ridge, TN 37830	FEWA (1983)	A two-dimensional finite-element model to simulate transient flow in confined, leaky confined, or water table aquifers.	leakage	3373
66.	D.N. Contractor Ref: 194	Water and Energy Research Institute of the Western Pacific University of Guam College Station, Mangilao, Guam 96913	SWIGS2D (1982)	A two-dimensional finite-element model to simulate transient, horizontal salt and fresh water flow separated by a sharp interface in an anisotropic, heterogeneous, confined, semi-confined or water table aquifer.	leakage	3600

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
67.	R.I. Allayla	Civil Engineering Department Colorado State University Fort Collins, CO 80523	SEAWTR/ SEACONF (1980)	A finite-difference model for two-dimensional horizontal simulation of simultaneous flow of salt and fresh water in a confined or water table aquifer with anisotropic and heterogeneous properties, including effects of capillary flow.	capillary forces influence capillary region on specific yield	3640
68.	I. Herrera J.P. Hennart R. Yates Ref: 68	Intituto De Geofisica Ciudad Universitaria 04510 Mexico, D.F.	LAFTID (1983)	A finite-element quasi-three-dimensional model for transient leaky aquifer flow including predictions of land subsidence.	consolidation leakage	3700
69.	F.T. Tracy Ref: 169	U.S. Army Engineer Waterways Experiment Station Automatic Data Processing Division P.O. Box 631 Vicksburg, MS 39180	ECPL 704-F3-RO-011 (1983)	A finite-element model for steady-state simulation of cross-sectional and axisymmetric flow in confined or unconfined, anisotropic, heterogeneous porous media.		3810
70.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	DFT/C-1D (1984)	A finite-element model for linear stress-deformation, and steady or transient fluid flow analysis of one-dimensional problems; calculation of displacement, fluid head, temperature or pore water pressure.	conduction consolidation campaction	3860
71.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	FIELD-2D	A finite-element model for linear steady analysis of two-dimensional problems in torsion, potential flow, seepage and heat flow.	conduction	3861
72.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	SEEP2(VM)-2D (1984)	A finite-element model for two-dimensional planar or axisymmetric simulation of steady confined, steady free surface and transient free surface seepage in structures such as dams, river banks, hillslopes and wells.		3862
73.	C.S. Desai Ref: 37	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	SEEP(VM)-3D (1983)	Three-dimensional simulation of confined, and steady and transient free surface seepage in porous bodies (dams, wells, slopes, drains, media with cracks), using a finite-element technique with variable and moving mesh.		3863

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
74.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	STRESEEP-2D (1984)	A finite-element model for combined stress, seepage and slope stability analysis of dams, embankments and slopes using the residual flow method.	consolidation	3864
75.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	CONS2-1D (1984)	A finite-element model for consolidation and settlement analysis of foundations idealized as one-dimensional with linear variation of pore water pressures.		3865
76.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	CONSP(L/NL)-2D (1984)	A finite-element model for consolidation and settlement analysis of foundations, dams and embankments idealized as plane strain.	consolidation	3866
77.	C.S. Desai	Department of Civil Engineering University of Arizona Tuscon, AZ 85721	CONSA(L)-2D (1984)	A finite-element model for consolidation and settlement analysis of foundations, piles, tanks and other structures, idealized as axisymmetric.	consolidation	3867
78.	D.G. Jorgensen H. Grubb C.H. Baker, Jr. G.E. Hilmes E.D. Jenkins Ref: 86	U.S. Geological Survey Water Research Dept. 1950 Ave. A-Campus West University of Kansas Lawrence, KS 66044-3897	GWMD3-APPROPRIATION MODEL (1982)	An axisymmetric finite-difference model to calculate drawdown due to a proposed well, at all existing wells in the section of the proposed well and in the adjacent 8 sections and to compare drawdowns with allowable limits.		3870
79.	J.V. Tracy Ref: 167	U.S. Geological Survey Water Resources Dept. National Center Reston, VA 22092	PARAMETER ESTIMATION PROGRAM (1980)	An automated calibration procedure to calculate transmissivities, vertical conductivities, storage coefficients and specific storages of confining layers in the head results from a quasi-three-dimensional flow system, using a finite-difference flow model as input.		3880
80.	W.I.M. Elderhorst	Institute for Applied Geosciences TNO/DGV P.O. Box 285 2600 AG Delft The Netherlands	INVERS (1983)	A direct inverse model to calculate hydraulic resistance of confining layers in a multi-layered aquifer with steady-state groundwater flow.		3950
81.	M.G. McDonald A.W. Harbaugh Ref: 107	Ground Water Branch, WRD U.S. Geological Survey WGS-MS 433 Reston, VA 22092	MODFLOW (1988)	A modular three-dimensional finite-difference groundwater model to simulate transient flow in anisotropic, heterogeneous, layered aquifer systems.	evapotranspiration drainage	3980

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
82.	C.R. Kolterman Ref: 95	Water Resources Center Desert Research Inst. University of Nevada System Reno, NV	GWUSER/ CONJUN (1983)	A combined simulation-optimization model to determine optimal pumping locations and rates for confined aquifer with or without artificial recharge or for conjunctive use of aquifer stream system; uses finite-differences and linear programming.	aquifer-stream interaction	4070
83.	A.I. El-Kadi Ref: 43	International Ground Water Modeling Center Holcomb Research Inst. Butler University 4600 Sunset Avenue Indianapolis, IN 46208	ST2D (1985)	This is a two-dimensional model to solve a stochastic gravity drainage problem via the Monte-Carlo technique. The flow problem is solved, using the finite-element technique.		4160
84.	D.N. Contractor S.M.A. El Didy A.S. Ansary Ref: 25	Department of Civil Engineering Universtiy of Arizona Tuscon, AZ 85721	MAQWF (1987)	A finite-element model for simulation of transient two-dimensional horizontal flow in a multiple aquifer system. The model provides velocities to be used as input for transport model.		4530
85.	P.R. Schroeder J.M. Morgan T.M. Walski A.C. Gibson Ref: 153	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Ave. Indianapolis, IN 46208	HELP (1987)	A water budget model for the Hydrologic Evaluation of Landfill Performance.	surface storage, runoff, infiltration, percolation, evapotranspiration, soil moisture storage, lateral drainage	4680
86.	P.K.M. van der Heijde Ref: 177	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	THWELLS (1988)	An analytical model to calculate drawdown or buildup in an isotropic homogeneous non-leaky confined aquifer with multiple pumping and injection wells.		6022
87.	P.K.M. van der Heijde Ref: 178	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	GWFLOW (1987)	A package of seven analytical solutions for groundwater flow problems. The package includes solutions for partial penetration, leaky confined systems, layered systems, groundwater mounding, and stream depletion due to pumping.	stream depletion, mounding, leakage	6023

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
88.	P.K.M. van der Heijde	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	THCVFIT (1987)	An interactive program to determine transmissivity and storage coefficient from pump test data. This model replaces traditional curve-fitting by a graphics routine to match the Theis well function with field drawdown data.		6025
89.	A. Verruijt Ref: 187	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	BASIC GWF (1987)	A finite-element model for analysis of plane, steady or unsteady groundwater flow in an isotropic, heterogeneous, confined or unconfined aquifer.		6030
90.	K.S. Rathod K.R. Rushton Ref: 142	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	RADFLOW (1984)	A finite-difference model for transient radial flow towards a well in a homogeneous, isotropic aquifer. RADFLOW allows for changing confined/unconfined conditions in time, and it can handle variable pumping schedules.		6064
91.	P.K.M. van der Heijde Ref: 180	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	TSSLEAK (1988)	A least-squares procedure for fitting the Hantush and Jacobs equations to experimental pump test data to obtain estimates for storage coefficient, transmissivity, leakage coefficient, and aquitard permeability.	leakage	6081
92.	M.A. Butt C.D. McElwee Ref: 21	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	VARQ (1986)	A program to calculate aquifer parameters by automatically fitting pump test data with Theis-type curve. The program allows for variable discharge rates during the test.		6082
93.	M.S. Beljin Ref: 10	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	PUMPTEST (1986)	An interactive, menu-driven program package to calculate transmissivity and storage coefficient from time-drawdown, distance-drawdown, or recovery pump test data. Jacob's method and regression analysis are applied to a user-specified portion of the data curve.		6382
94.	L.A. Abriola G.F. Pinder Ref: 1	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	TETRA (1985)	A simple program to calculate velocity components in three dimensions from hydraulic head measurements.		6430

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
95.	K.R. Bradbury E.R. Rothschild Ref: 17	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	TGUESS (1986)	A program for estimating transmissivity from specific capacity data. TGUESS corrects for partial penetration and well loss.		6450
96.	D.B. Thompson Ref: 166	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	TIMELAG (1987)	A program to estimate hydraulic conductivity from time-lag slug tests.		6580
97.	J.M. Shafer Ref: 158	Illinois State Water Survey Ground Water Section 2204 Griffith Drive Champaign, IL 61820-7495	GWPATH (1987)	An interactive software package for estimating horizontal fluid pathlines and traveltimes in fully saturated media. GWPATH is applicable to heterogeneous anisotropic flow systems, and it features forward and reverse pathline tracking, time-related capture zone analysis, and multiple pathline capture detection mechanisms.	nonuniform flow	6650

APPENDIX A2 SATURATED FLOW MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
1.	S.P. Neuman P.A. Witherspoon	FREESURF I	Y	G	Y	Y	N	Y	Y	Y	Y	L	M	0020
2.	S.P. Neuman P.A. Witherspoon	FREESURF II	U	U	Y	Y	L	N	Y	U	Y	U	U	0022
3.	T.R. Narasimhan	TERZAGI	U	U	Y	Y	N	L	Y	Y	Y	Y	M	0121
4.	R.L. Cooley J. Peters	ECPL 723-62-L2440	N	N	Y	Y	L	N	Y	U	Y	Y	F	0140
5.	R.L. Cooley J. Peters	Steady-State Finite Element Solution	U	U	Y	Y	Y	N	Y	U	Y	Y	U	0141
6.	R.L. Cooley	Non-Linear Regression Groundwater Flow Model	U	U	Y	Y	L	Y	Y	Y	Y	Y	F	0195
7.	H.J. Morel-Seytoux, et al.	DELTA	U	U	Y	Y	Y	Y	Y	U	Y	L	F	0260
8.	T.A. Prickett C.G. Lonnquist	PLASM	D	G	Y	Y	N	Y	Y	Y	Y	L	M	0322
9.	G.F. Pinder E.O. Frind	ISOQUAD	U	G	Y	Y	N	Y	Y	U	Y	L	U	0510
10.	G.F. Pinder	AQUIFEM	N	G	Y	Y	N	Y	Y	U	Y	L	F	0514
11.	P.S. Huyakorn	STAFAN2	N	N	Y	Y	L	Y	Y	U	Y	U	F	0584
12.	T.R. Knowles	GSWIM	U	U	Y	Y	Y	Y	Y	U	U	L	U	0681
13.	C.R. Faust, et al.	STFLO	U	U	Y	Y	N	U	U	U	Y	U	U	0694
14.	S.B. Pahwa B.S. Rama Rao	NETFLO	U	U	Y	Y	Y	Y	Y	U	Y	U	F	0695

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			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
15.	T. Maddock, III	Leaky Aquifer Simulation	U	U	Y	Y	L	N	U	U	U	L	U	0756
16.	P.C. Trescott S.P. Larson	USGS-3D-FLOW	N	N	Y	Y	N	Y	Y	Y	Y	L	M	0770
17.	P.C. Trescott G.F. Pinder S.P. Larson	USGS-2D-FLOW	N	N	Y	Y	N	Y	Y	Y	Y	L	M	0771
18.	V. Guvanasen	IDPNGM	U	U	Y	Y	U	N	U	U	Y	Y	F	0951
19.	K.R. Rushton L.M. Tomlinson	AGU-1	U	U	Y	Y	N	Y	Y	Y	Y	Y	M	1230
20.	M. Clouet D'Orval	BURGEAP 7600 HYSO PACKAGE	N	N	Y	Y	Y	N	U	U	Y	Y	M	1370
21.	M. Clouet D'Orval	TRABISA	N	N	Y	Y	Y	N	U	U	U	Y	M	1371
22.	M. Clouet D'Orval	TRABICO	N	N	Y	Y	Y	N	U	U	U	Y	M	1372
23.	A. Levassor	PLIN	U	U	Y	Y	L	N	U	U	Y	Y	F	1470
24.	P. Prudhomme, et al.	BIDAT-HS2	U	U	Y	Y	L	N	U	U	Y	Y	M	1481
25.	P. Prudhomme, et al.	TRIGAT-HS1 OR AXYZ-HS5	U	U	Y	Y	L	N	U	U	Y	Y	M	1482
26.	B. Boehm	GW1	U	U	Y	Y	L	Y	Y	U	Y	Y	F	1531
27.	Y. Bachmat A. Dax	Inverse Multicell Aquifer Model	U	U	Y	Y	Y	N	Y	U	U	Y	F	1631
28.	D.A. Blank	AQSIM	U	U	Y	Y	L	N	Y	U	Y	Y	F	1651
29.	H.M. Haitjema O.D.L. Strack	SYLENS	D	D	Y	Y	Y	Y	Y	U	Y	Y	F	1791

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			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
30.	T.N. Olsthoorn	TOFEM-N	U	U	Y	Y	Y	Y	Y	U	Y	Y	F	1814
31.	C. van der Akker	FLOP	U	U	Y	Y	N	N	U	U	U	Y	F	1820
32.	C. van der Akker	FLOP-2	U	U	Y	Y	N	Y	Y	U	Y	Y	M	1821
33.	C. van der Akker	FRONT	U	U	Y	Y	L	Y	Y	U	Y	Y	M	1822
34.	P. van der Veer	MOTGRO	U	U	Y	Y	N	Y	Y	U	Y	L	F	1830
35.	A. Verruijt J.B.S. Gan	SWIFT	U	U	Y	Y	N	Y	Y	U	Y	U	F	1852
36.	D.E. Evenson	PEP	U	U	Y	Y	Y	N	Y	U	Y	Y	F	1940
37.	K. Ueshita K. Sato	CONSOL-1	U	U	Y	Y	U	Y	Y	U	Y	L	F	2021
38.	H.J. Morel-Seytoux T. Illangasekare	DELTIS	U	U	Y	Y	Y	N	Y	U	Y	U	F	2060
39.	H.J. Morel-Seytoux, et al.	DELPET	U	U	Y	Y	Y	N	Y	U	Y	L	F	2061
40.	S.K. Gupta, et al.	FE3DGW	D	D	Y	Y	Y	Y	Y	Y	Y	Y	M	2072
41.	A.E. Reisenauer C.R. Cole	VTTSS3	U	U	Y	Y	Y	N	Y	U	Y	Y	F	2090
42.	A.E. Reisenauer C.R. Cole	VTTSS2	U	U	Y	Y	Y	N	Y	U	Y	Y	F	2091
43.	A.E. Reisenauer C.R. Cole	VTT	Y	Y	Y	Y	Y	Y	U	U	Y	Y	M	2092
44.	J.W. Mercer C.R. Faust	SWSOR	U	U	Y	Y	L	Y	Y	U	Y	Y	F	2140
45.	J.B. Weeks	Quasi 3-D Multiaqui-fer Model	U	U	Y	Y	L	N	Y	U	Y	Y	F	2510
46.	L.R. Townley, et al.	AQUIFEM-1	N	G	Y	Y	N	Y	Y	U	Y	L	M	2630

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			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
47.	L.K. Kuiper	Variable Density Model	U	U	Y	Y	U	N	Y	U	Y	L	F	2663
48.	R.H. Page	INTERFACE	U	U	Y	Y	L	N	Y	U	Y	L	F	2720
49.	D.R. Posson, et al.	N.M.F.D. 3D	U	U	Y	Y	Y	Y	Y	U	Y	L	F	2740
50.	C.J. Daly	CRREL	U	Y	Y	Y	Y	Y	Y	U	Y	L	F	2791
51.	J. Boonstra	SGMP	N	U	Y	Y	N	Y	Y	U	Y	U	F	2800
52.	O. Berney	DISIFLAQ	N	N	Y	Y	N	Y	U	U	Y	U	M	2870
53.	H.N. Tyson, et al.	KRGW	U	U	Y	Y	U	N	Y	U	U	Y	F	2930
54.	A.P.M. Broks, et al.	GROMULA	U	U	Y	Y	Y	Y	Y	U	Y	L	F	2980
55.	B.H. Gilding J.W. Wesseling	GROMAGE	U	U	Y	Y	Y	Y	Y	U	Y	L	F	2981
56.	J. Noorishad P.A. Witherspoon	ROCMAS-H	U	U	Y	Y	U	N	Y	U	Y	U	U	3080
57.	J. Noorishad et al.	ROCMAS-HM	U	U	Y	Y	U	N	Y	U	Y	U	U	3082
58.	G. Schmid	SICK 100	U	Y	Y	Y	L	Y	Y	Y	Y	L	U	3110
59.	P.M. Cobb, et al.	TSSLEAK	U	U	Y	Y	L	Y	Y	Y	Y	Y	U	3160
60.	B. Sagar	AQUIFER	U	U	Y	Y	N	U	U	U	Y	L	U	3230
61.	B. Sagar	DEWATER	U	U	Y	Y	N	Y	Y	U	Y	L	Y	3231
62.	J.A. Liggett	GM5	N	N	Y	Y	N	N	Y	N	Y	L	F	3240
63.	P.J.T. van Badel	FEMSAT	U	U	Y	Y	L	Y	U	U	Y	L	F	3350
64.	G.T. Yeh C.W. Francis	AQUIFLOW	N	G	Y	Y	N	Y	U	U	Y	L	U	3372
65.	G.T. Yeh D.D. Huff	FEWA	N	G	Y	Y	N	Y	U	U	Y	L	F	3373
66.	D.N. Contractor	SWIGS2D	U	U	Y	Y	U	Y	Y	U	Y	L	F	3600

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67.	R.I. Allayla	SEAWTR/ SEACONF	Y	Y	Y	Y	U	N	Y	U	Y	U	L	3640
68.	I. Herrera, et al.	LAFT1D	U	U	Y	Y	Y	Y	Y	Y	Y	Y	F	3700
69.	F.T. Tracy	ECPL 704-F3-RO-011	U	D	Y	Y	U	Y	Y	U	Y	L	F	3810
70.	C.S. Desai	DFT/C-1D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3860
71.	C.S. Desai	FIELD-2D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3861
72.	C.S. Desai	SEEP2(VM)-2D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3862
73.	C.S. Desai	SEEP(VM)-3D	U	U	Y	Y	L	Y	Y	U	Y	L	U	3863
74.	C.S. Desai	STRESEEP-2D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3864
75.	C.S. Desai	CONS2-1D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3865
76.	C.S. Desai	CONSP (L/NL)-2D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3866
77.	C.S Desai	CONSA(L)-2D	U	U	Y	Y	U	Y	Y	U	Y	L	U	3867
78.	D.G. Jorgensen, et al.	GWMD3	N	U	Y	Y	N	Y	Y	U	Y	L	U	3870
79.	J.V. Tracy	Parameter Estimation Program	U	U	Y	Y	U	N	U	U	U	L	U	3880
80.	W.I.M. Elderhorst	INVERS	U	U	Y	Y	Y	Y	U	U	U	L	U	3950
81.	M.G. McDonald A.W. Harbaugh	MODFLOW	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	M	3980
82.	C.R. Kolterman	GWUSER/ CONJUN	U	U	Y	Y	Y	Y	U	U	Y	L	U	4070
83.	A.I. El-Kadi	ST2D	N	N	Y	Y	L	Y	Y	U	Y	L	U	4160
84.	D.M. Contractor, et al.	MAQWF	U	U	Y	Y	Y	N	Y	U	U	U	U	4530

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			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
85.	P.R. Schroeder, et al.	HELP	D	N	Y	Y	N	Y	U	U	U	U	M	4680
86.	P.K.M. van der Heijde	THWELLS	D	D	Y	Y	L	Y	Y	N	Y	L	M	6022
87.	P.K.M. van der Heijde	GWFLOW	D	N	Y	Y	N	Y	U	N	Y	L	M	6023
88.	P.K.M. van der Heijde	THCVFIT	D	D	Y	Y	L	Y	U	U	Y	L	M	6025
89.	A. Verruijt	BASIC GWF	D	N	N	N	U	L	Y	U	U	U	F	6030
90.	K.S. Rathod K.R. Rushton	RADFLOW	D	N	Y	Y	U	Y	Y	U	Y	L	M	6064
91.	P.K.M. van der Heijde	TSSLEAK	D	D	Y	Y	L	Y	Y	N	Y	L	M	6081
92.	M.A. Butt	VARQ	D	N	Y	Y	N	Y	U	U	Y	L	M	6082
93.	M.S. Beljin	PUMPTEST	D	D	Y	Y	L	Y	Y	N	Y	L	M	6382
94.	L.A. Abriola G.F. Pinder	TETRA	D	N	Y	Y	U	Y	Y	U	Y	L	M	6430
95.	K.R. Bradbury E.R. Rothschild	TGUESS	D	N	Y	Y	N	Y	U	U	Y	L	M	6450
96.	D.B. Thompson	TIMELAG	D	D	Y	Y	L	L	Y	U	Y	U	F	6580
97.	J.M. Shafer	GWPATH	D	D	Y	Y	L	L	U	U	Y	U	F	6650

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APPENDIX B1 VARIABLY SATURATED FLOW MODELS: SUMMARY LISTING

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	S.P. Neuman Ref: 31	Dept. of Hydrology and Water Resources Univ. of Arizona Tuscon, AZ 85721	UNSAT2 (1979)	A two-dimensional finite-element model for horizontal, vertical or axisymmetric simulation of transient flow in a variably saturated, non-uniform, anisotropic porous medium.	capillarity evapo-transpiration plant uptake	0021
2.	T.N. Narasimhan Ref: 145	Water and Land Resources Division Battelle Pacific NW Lab P.O. Box 999 Richland, WA 99352	TRUST (1981)	To compute steady and nonsteady pressure head distributions in multi-dimensional, heterogeneous, variably saturated, deformable porous media with complex geometry; uses integrated-finite-differece method.	capillarity diffusion consolidation hysteresis	0120
3.	T.N. Narasimhan S.P. Neuman Ref: 113	Earth Sciences Division Lawrence Berkeley Laboratory University of California Berkeley, Ca 94720	FLUMP (1981)	A finite-element model for computation of steady and nonsteady pressure head distributions in two-dimensional or axisymmetric, heterogeneous, anisotropic, variably saturated porous media with complex geometry.	capillarity diffusion evapo-transpiration	0122
4.	A. Vandenberg Ref: 176	National Hydrology Research Institute Inland Waters Directorate Ottawa, K1A 0E7 Ontario, Canada	FLO (1985)	FLO simulates the elements of the hydrologic cycle which are directly influenced by soil and surface drainage improvements. Total discharge from a drained plot is estimated. Detailed accounts of unsaturated flow are considered.	capillarity evapo-transpiration	1092
5.	P.J.M. DeLaat Ref: 35	International Inst. for Hydraulic and Environm. Eng. Delft, The Netherlands	MUST (1985)	A finite-difference model which simulates one-dimensional vertical, unsaturated groundwater flow, evapo-transpiration, and interception of precipitation by plants.	capillarity evapo-transpiration plant uptake	1771
6.	R. W. Skaggs Ref: 159	P.O. Box 5906 Dept. of Biological and Agricultural Eng. North Carolina State University Raleigh, NC 27650	DRAINMOD (1980)	An analytical model for unsteady, one-dimensional, horizontal/vertical, saturated/unsaturated problems; simulates water table position and soil water regime above water table for artificially drained soils.	capillarity evapo-transpiration	1950

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No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
7.	D.L. Ross H.J. Morel-Seytoux Ref: 146	Dept. of Civil Eng. Colorado State Univ. Fort Collins, CO 80523	SOILMOP (1982)	An analytical model to predict ponding time, infiltration rate and amount, and water content profiles under variable rainfall conditions. The model solves a one-dimensional flow equation in a homogeneous soil. Air phase is also included.	capillarity	2062
8.	S.K. Gupta C.S. Simmons Ref: 60	Battelle Pacific NW Labs P.O. Box 999 Richland, WA 99352	UNSAT1D (1981)	A finite-difference model for one-dimensional simulation of unsteady vertical unsaturated flow.	capillarity evapo-transpiration plant uptake	2071
9.	R.A. Feddes Ref: 11	Inst. for Land and Water Management Research P.O. Box 35 6700 AA Wageningen The Netherlands	SWATRE, SWATR-CROPR (1981)	A finite-difference model for simulation of the water balance of agricultural soil.	precipitation capillarity evapo-transpiration	2550
10.	L.A. Davis Ref: 32	Water, Waste and Land, Inc. 1311 S. Collins Ave. Fort Collins, CO 80524	SEEPV (1980)	A finite-difference transient flow model to simulate vertical seepage from a tailings impoundment in variably saturated flow systems; considers interactions between a liner and the underlying aquifer.	infiltration capillarity evapo-transpiraton	2890
11.	J.W. Wesseling	Delft Hydraulics Laboratory P.O. Box 152 8300 AD Emmeloord The Netherlands	SOMOF (1982)	A finite-difference model for simulation of transient unsaturated soil moisture flow in a vertical profile.	precipitation capillarity evapo-transpiration gravity drainage plant uptake ponding	2983
12.	G.T. Yeh D.S. Ward Ref: 195	Environmental Sciences Division Oak Ridge National Lab Oak Ridge, TN 37830	FEMWATER/ FECWATER (1987)	A two-dimensional finite-element model to simulate transient, cross-sectional flow in saturated-unsaturated anisotropic, heterogenous porous media.	capillarity infiltration, ponding	3370
13.	G.T. Yeh R.J. Luxmoore Ref: 198	Environmental Sciences Division Oak Ridge National lab Oak Ridge, TN 37830	MATTUM (1983)	This is a three-dimensional model for simulating moisture and thermal transport in unsaturated porous media. The model solves both the flow equation and the heat equation under unsaturated water conditions, using the integrated compartment method.	capillarity	3375
14.	J.L. Neiber Ref: 118	Dept of Agricultural Eng Cornell University Ithaca, New York 14853	FEATSMF (1979)	A transient finite-element 2-D soil moisture flow model for homogeneous, isotropic hillslopes where the moisture is supplied by rainfall.	capillarity evapo-transpiration	3420

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
15.	M. Th. van Genuchten Ref: 182	U.S. Salinity Lab U.S. Dept. of Agriculture 4500 Glenwood Drive Riverside, CA 92501	UNSAT1 (1978)	A finite-element solution to Richards' equation to simulate one-dimensional saturated-unsaturated flow in heterogeneous soils.	capillarity evapo-transpiration	3431
16.	J.B. Kool J.C. Parker M.Th. van Genuchten Ref: 97	245 Smyth Hall Va. Polytechnic Inst. Blacksburg, VA. 24061	ONESTEP (1985)	A nonlinear parameter estimation model for evaluating soil hydraulic properties from one-step outflow experiments in one-dimensional flow.	capillarity	3433
17.	M. Vauclin Ref: 40	Institute De Mecanique De Grenoble - BP 68 38402 St. Martin D'Heres - Cedex, France	INFIL (1983)	The finite-difference model solves for one-dimensional infiltration into a deep homogeneous soil. Output includes water content profile and amount and rate of infiltration at different simulation times.	capillarity infiltration evapo-transpiration	3570
18.	P. Christopher D. Milly Ref: 110	Dept. of Civil Eng. Princeton University Princeton, NJ 08544	SPLASHWATR (1983)	Simulation of coupled heat and moisture fields in the unsaturated zone.	capillarity evapo-transpiraton convection conduction diffusion change of phase hysteresis adsorption	3590
19.	D.K. Sunada Ref: 88	Dept. Civil Eng. Colorado State University Fort Collins, CO 80523	GRWATER (1981)	A finite-difference model to predict the decline of ground-water mounds developed under recharge in an isotropic, heterogeneous aquifer with transient saturated or unsaturated flow conditions.	infiltration capillarity evapo-transpiration	3660
20.	M.J. Fayer G.W. Gee Ref: 50	Battelle Pacific Northwest Lab Richland, WA 99352	UNSAT-H (1985)	UNSAT-H is a finite-difference one-dimensional, unsaturated flow model. It simulates infiltration, drainage, redistribution, surface evaporation, and plant water uptake from soil. The model is designed for arid zones similar to the Hanford Site (Washington).	capillarity evapo-transpiration infiltration drainage plant uptake	4340
21.	P.M. Craig E.C. Davis Ref: 28	Environmental Science Division Oak Ridge Nat'l. Laboratory Oak Ridge, TN	INFGR (1985)	1-D vertical model to estimate infiltration rates, using the Green and Ampt equation. The compression method is used to estimate infiltration during low rainfall periods.	capillarity	4380

APPENDIX B1 VARIABLY SATURATED FLOW MODELS: SUMMARY LISTING

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
22.	R-M Li K.G. Eggert K. Zachmann Ref: 102	Simons, Li, & Associates, Inc. P.O. Box 1816 Fort Collins, CO 80522	FLOWVEC (1983)	A finite-difference model which utilizes a vector processor for solutions to three-dimensional variably saturated flow problems.	capillary forces	4390
23.	G.P. Korfiatis Ref: 98	Civil and Environmental Engineering Rutgers University The State University of New Jersy New Brunswick, NJ	LANDFIL (1984)	Model simulates the transport of moisture through the unsaturated zone, using a finite-difference solution for the 1-D flow equation.	capillarity evapotranspiration	4400
24.	E.R. Perrier A.C. Gibson Ref: 129	Solid and Hazardous Waste Research Div. Municipal Environmental Research Laboratory Cincinnati, OH 45268	HSSWDS (1982)	1-D analytical water budget model to estimate the amount of moisture percolation through different types of landfills.	capillarity evapotranspiration runoff snowmelt	4410
25.	E.G. Lappala R.W. Healy E.P. Weeks Ref: 100	U.S. Geological Survey Box 25046, M.S. 413 Denver Federal Center Denver, CO 80225	VS2D (1987)	2-D finite-difference code for the analysis of flow in variably saturated porous media. Model considers recharge, evaporation, and plant root uptake.	evaporation recharge plant uptake	4570
26.	A.I. El-Kadi Ref: 42	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	SOIL (1987)	A model to estimate soil hydraulic properties, using a non-linear least squares analysis.		6330
27.	A.I. El-Kadi Ref: 41	International Ground Water Modeling Center Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	INFIL (1987)	An analytical solution to calculate infiltration rate and water content profile at different times, using the Philip series solution of a one-dimensional form of the Richards equation.	infiltration	6335
28.	D.L. Nofziger Ref: 121	Institute of Food and Agricultural Sciences University of Florida Gainesville, FL 32611	WATERFLO (1985)	A one-dimensional finite-difference solution for the Richards equation to simulate water movement through soils.		6630

APPENDIX B2 VARIABLY SATURATED FLOW MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
1.	S.P. Neuman	UNSAT2	Y	G	Y	Y	L	Y	Y	Y	Y	L	M	0021
2.	T.N. Narasimhan	TRUST	U	D	U	U	N	Y	Y	U	Y	L	F	0120
3.	T.N. Narasimhan S.P. Neuman	FLUMP	U	U	Y	Y	U	U	Y	Y	Y	L	F	0122
4.	A. Vandenberg	FLO	U	U	Y	Y	Y	N	U	U	U	U	F	1092
5.	P.J.M. DeLaat	MUST	U	U	Y	Y	U	Y	Y	U	Y	L	F	1771
6.	R.W. Skaggs	DRAINMOD	U	U	Y	Y	Y	N	Y	U	Y	Y	F	1950
7.	D.L. Ross H.J. Morel-Seytoux	SOILMOP	U	U	Y	Y	Y	N	U	U	U	U	F	2062
8.	S.K. Gupta C.S. Simons	UNSAT1D	U	U	Y	Y	Y	Y	Y	U	Y	Y	F	2071
9.	R.A. Feddes	SWATRE SWATR-CROPR	U	U	Y	Y	Y	N	Y	U	Y	L	F	2550
10.	L.A. Davis	SEEPV	U	U	Y	Y	Y	N	Y	U	Y	L	F	2890
11.	J.W. Wesseling	SOMOF	U	U	Y	Y	Y	Y	Y	U	Y	Y	F	2983
12.	D.W. Green H. Dabiri C.F. Wienaug R. Prill	TWO-PHASE UNSATURATED FLOW	N	N	Y	Y	Y	N	N	N	Y	Y	F	3280
13.	G.T. Yeh D.S. Ward	FEMWATER/ FECWATER	N	G	Y	Y	N	Y	Y	Y	Y	Y	M	3370
14.	G.T. Yeh R.J. Luxmoore	MATTUM	U	U	Y	U	N	Y	U	U	Y	U	F	3375
15.	J.L. Neiber	FEATSMF	U	U	Y	Y	Y	N	Y	U	Y	L	F	3420
16.	M.Th. van Genuchten	UNSAT1	U	U	Y	Y	N	Y	Y	Y	Y	L	M	3431

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

APPENDIX B2 VARIABLY SATURATED FLOW MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
17.	J.B. Kool J.C. Parker M.Th. van Genuchten	ONESTEP	U	U	Y	Y	N	Y	Y	Y	Y	L	F	3433
18.	M. Vauclin	INFIL	N	N	Y	Y	Y	Y	Y	Y	Y	L	F	3570
19.	P. Christopher D. Milly	SPLASHWATR	U	U	Y	Y	Y	Y	Y	U	Y	Y	F	3590
20.	D.K. Sunada	GRWATER	U	U	Y	Y	Y	N	Y	U	Y	L	F	3660
21.	M.J. Fayer G.W. Gee	UNSAT-H	U	U	Y	Y	Y	N	Y	U	Y	L	F	4340
22.	E.C. Davis	INFGR	U	U	Y	Y	Y	U	U	U	U	L	F	4380
23.	R-M Li	FLOWVEC	U	U	Y	Y	U	Y	U	U	Y	U	F	4390
24.	G.P. Korfiatis	LANDFIL	U	U	Y	Y	Y	N	Y	U	Y	U	F	4400
25.	R.E. Landreth	HSSWDS	U	U	Y	Y	N	N	Y	U	Y	U	F	4410
26.	E.G. Lappala R.W. Healy E.P. Weeks	VS2D	U	U	Y	Y	Y	N	N	N	U	U	F	4570
27.	A.I. El-Kadi	SOIL	D	D	Y	Y	L	Y	Y	N	Y	L	M	6330
28.	A.I. EL-Kadi	INFIL	D	D	Y	Y	L	Y	Y	N	Y	L	M	6335
29.	D.L. Nofziger	WATERFLO	D	D	Y	Y	L	U	U	U	U	U	F	6630

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

APPENDIX C1 SOLUTE TRANSPORT MODELS: SUMMARY LISTING

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	P.S.C. Rao Ref: 30	2169 McMarthy Hall Soil Science Dept. University of Florida Gainesville, FL 32611	NITROSIM (1981)	A finite-difference solution for simulation of transport and plant uptake of nitrogen and transformations of nitrogen and carbon in the root zone.	capillarity precipitation evapo-transpiration convection dispersion diffusion adsorption ion exchange decay	0280
2.	H.M. Selim J.M. Davidson Ref: 154	Louisiana Agricultural Experiment Station Agronomy Dept. Louisiana State Univ. Baton Rouge, LA 70803	NMODEL (1976)	A finite-difference model for steady or unsteady simulation of one-dimensional, vertical water and nitrogen transport and nitrogen transformations in unsaturated multilayered homogeneous soils.	capillarity convection dispersion diffusion adsorption nitrification plant uptake	0290
3.	G.F. Pinder Ref: 133	Dept. of Civil Eng. Princeton Univ. Princeton, NJ 08540	ISOQUAD 2 (1977)	A finite-element model to solve the transport equation in nonsteady, confined, areal, two-dimensional groundwater flow systems.	advection dispersion diffusion	0511
4.	P. Huyakorn Ref: 78	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	TRAFRAP-WT (1987)	A finite-element model to study transient, two-dimensional, saturated ground water flow and chemical or radionuclide transport in fractured and unfractured, anisotropic, heterogeneous, multilayered porous media.	advection dispersion diffusion adsorption decay chemical reactions	0589
5.	P. Huyakorn Ref: 70	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	GREASE2 (1982)	A finite-element model to study transient, multidimensional, saturated ground water flow, solute and/or energy transport in fractured and unfractured, anisotropic, heterogeneous, multilayered porous media.	advection conduction dispersion diffusion buoyancy adsorption	0582
6.	P. Huyakorn Ref: 75	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	SATURN2 (1982)	A finite-element model to study transient, two-dimensional variably saturated flow and solute transport in anisotropic, heterogeneous porous media.	advection conduction dispersion diffusion adsorption decay chemical reactions	0583
7.	P. Huyakorn Ref: 72	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	SEFTRAN (1985)	A two-dimensional finite-element model for simulation of transient flow and transport of heat or solutes in anisotropic, heterogeneous porous media.	advection dispersion diffusion adsorption decay	0588

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
8.	T.R. Knowles Ref: 163	Texas Dept. of Water Res P.O. Box 13087 Capitol Station Austin, TX 78758	GWSIM-II (1981)	A transient, two-dimensional, horizontal model for prediction of water levels and water quality in an anisotropic, heterogeneous, confined or unconfined aquifer based on finite-difference method.	advection dispersion diffusion	0680
9.	INTERA Environmental Consult., Inc. Ref: 84	K. Kipp U.S.. Geological Survey Box 25046, mail Stop 411 Denver Federal Center Lakewood, CO 80225	SWIPR (1985)	A finite-difference model to simulate nonsteady, three-dimensional ground water flow and heat and contaminant transport in a heterogeneous aquifer.	advection conduction dispersion diffusion adsorption	0692
10.	L.F. Konikow J.D. Bredehoeft Ref: 96	L.F. Konikow U.S. Geological Survey 12201 Sunrise Valley Dr. Reston, VA 22092	USGS-2D-TRANSPORT/MOC (1988)	To simulate transient, two-dimensional, horizontal ground water flow and solute transport in confined/semiconfined aquifers using finite differences and method of characteristics.	advection dispersion diffusion adsorption decay	0740
11.	S.P. Garabedian L.F. Konikow Ref: 53	L.F. Konikow Water Resources Division U.S. Geological Survey 12201 Sunrise Valley Dr. Reston, VA 22092	FRONTTRACK (1983)	A finite-difference model for simulation of convective transport of a conservative tracer dissolved in groundwater under steady or transient flow conditions. The model calculates heads, velocities and tracer particle positions.	advection	0741
12.	S.W. Ahlstrom H.P. Foote R.J. Serne Ref: 2	Battelle Pacific NW Laboratories P.O. Box 999 Richland, WA 99352	MMT-DPRW (1976)	To predict the transient three-dimensional movement of radionuclides and other contaminants in unsaturated/saturated aquifer systems.	convection dispersion adsorption absorption ion exchange decay reactions	0780
13.	F.E. Kaszeta C.S. Simmons C.R. Cole Ref: 192	Battelle Pacific NW Labs P.O. Box 999 Richland, WA 99352	MMT-1D (1980)	A finite-difference model to simulate transient, one-dimensional movement of radionuclides and other contaminants in saturated/unsaturated aquifer systems.	capillarity convection dispersion adsorption absorption ion exchange decay	0781
14.	V. Guvanasen Ref: 24	Applied Geoscience Branch Whiteshell Nuclear Research Atomic Energy of Canada Pinawa, Manitoba ROE1I0	MOTIF (1986)	Finite-element model for one, two, and three-dimensional saturated/unsaturated groundwater flow, heat transport, and solute transport in fractured porous media; facilitates single-species radionuclide transport and solute diffusion from fracture to rock matrix.	convection dispersion diffusion adsorption decay advection	0953

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
15.	I. Miller J. Marlon-Lambert Ref: 105	Golder Associates 2950 Northup Way Bellevue, WA 98004	Golder Groundwater Computer Package (1983)	A transient finite-element model to simulate hydraulic and solute transport characteristics of two-dimensional, horizontal or axi-symmetric ground water flow systems with layered geometry.	advection dispersion diffusion adsorption decay chemical reaction	1010
16.	S.K. Gupta C.T. Kinkaid P.R. Meyer C.A. Newbill C.R. Cole Ref: 59	C.R. Cole Battelle Pacific NW Labs P.O. Box 999 Richland, WA 99352	CFEST (1987)	A three-dimensional finite-element model to simulate coupled transient flow, solute- and heat-transport in saturated porous media.	advection dispersion diffusion adsorption decay	2070
17.	H.C. Burkholder M.O. Cloninger W.V. Demier G. Jansen P.J. Liddell J.F. Washburn Ref: 36	Natl. Energy Software Center Argonne Natl. Laboratory 9700 S. Cass Avenue Argonne, IL 60439	GETOUT (1979)	A one-dimensional analytical model for radionuclide transport.	advection dispersion diffusion adsorption ion exchange (chain) decay	2080
18.	R.W. Nelson Ref: 114	Battelle Pacific NW Labs P.O. Box 999 Richland, WA 99352	PATHS (1980)	To evaluate contamination problems in unsteady, two-dimensional ground water flow systems, using an analytical solution for the flow equation and the Runge-Kutta method for the pathline equation.	advection adsorption ion exchange	2120
19.	R.D. Schmidt Ref: 157	U.S. Dept. of the Interior Bureau of Mines P.O. Box 1660 Twin Cities, MN 55111	ISL-50 (1979)	A three-dimensional semi-analytical model to describe transient flow behavior of leachates and ground water, involving an arbitrary pattern of injection and recovery wells.	advection	2560
20.	T.A. Prickett T.G. Naymik C.G. Lonnquist Ref: 138	Ill. State Water Survey P.O. Box 5050, Sta. A Champaign, IL 61820	Random Walk (1981)	To simulate one- or two-dimensional, steady/non-steady flow and solute transport problems in a heterogeneous aquifer with water table and/or confined or semiconfined conditions, using a "random-walk" technique.	advection dispersion diffusion adsorption decay chemical reaction	2690
21.	B. Ross C.M. Koplik Ref: 4	Analytic Sciences Corp. Energy & Environment Div. One Jacob Way Reading, MA 01867	WASTE (1981)	An analytical solution to compute one- or two-dimensional horizontal, or one-dimensional vertical, steady/unsteady transport of radionuclides in confined or semiconfined, anisotropic, heterogeneous multi-aquifer systems.	advection dispersion diffusion adsorption ion exchange decay	2810

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
22.	L.A. Davis G. Segol Ref: 33	Water, Waste and Land, Inc. 1311 S. College Avenue Fort Collins, CO 80524	GS2 (1985)	GS2 is a two-dimensional finite-element code for the analysis of flow and contaminant transport in partially saturated media. Either vertical or horizontal plane simulation is possible. Mass transport analysis includes convection, dispersion, radioactive decay, adsorption.	evapo-transpiration convection dispersion diffusion adsorption decay infiltration	2891
23.	L.A. Davis G. Segol Ref: 33	Water, Waste, and Land, Inc. 1311 S. College Avenue Fort Collins, CO 80524	GS3 (1985)	GS3 is a three-dimensional finite-element code for analysis of fluid flow and contaminant transport in partially saturated media. The code is particularly useful for simulation of anisotropic systems with strata of varying thickness and continuity.	evapo-transpiration convection dispersion diffusion infiltration	2892
24.	J.W. Wesseling	Delft Hydraulics Lab. P.O. Box 152 8300 AD Emmeloord The Netherlands	GROWKWA (1982)	Transient finite-element simulation of two-dimensional, horizontal ground water flow and transport of nonconservative solutes in a multi-layered, anisotropic, heterogeneous aquifer system.	advection dispersion diffusion adsorption ion exchange decay chemical reactions	2982
25.	J. Noorishad M. Mehran Ref: 123	Earth Sciences Division Lawrence Berkeley Lab. Univ. of California Berkeley, CA 94720	ROCMAS-HS (1981)	A transient finite-element model to solve for two-dimensional dispersive-convective transport of non-conservative solutes in saturated, fractured porous media for a given velocity field as generated by ROCMAS-H.	convection dispersion diffusion adsorption decay reactions	3081
26.	J.W. Warner Ref: 191	Civil Engineering Dept. Colorado State Univ. Ft. Collins, CO 80523	RESTOR (1981)	A finite-element model to calculate the dual changes in concentration of two reacting solutes subject to binary cation exchange in flowing ground water; two-dimensional simulation of areal transient or steady ground water flow and transient coupled transport of two solutes in an anisotropic, heterogeneous confined aquifer.	advection dispersion diffusion ion-exchange	3100
27.	S. Haji-Djafari T.C. Wells Ref: 67	D'Appolonia Waste Mngmt. Services, Inc. 10 Duff Rd. Pittsburgh, PA 15235	GEOFLOW (1982)	A three-dimensional finite-element model to simulate coupled transient flow, solute- and heat-transport in saturated porous media.	advection dispersion diffusion	3220

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
28.	B. Sagar Ref: 52	Analytic & Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	FRACFLOW (1981)	An integrated-finite-difference approach for steady and unsteady state analysis of density-dependent flow, heat and mass transport in fractured confined aquifers. Two-dimensional simulation of the processes in the porous medium and one-dimensional simulation of the fractures.	convection conduction dispersion diffusion consolidation adsorption decay reactions	3232
29.	A.K. Runchal Ref: 46	Analytic & Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	PORFLOW II & III (1988)	An integrated-finite-difference model for steady or transient, 2-D horizontal, vertical or radial and 3-D simulation of density-dependent flow, heat and mass transport in anisotropic, heterogeneous, nondeformable saturated porous media with time-dependent aquifer and fluid properties.	convection conduction dispersion diffusion change of phase adsorption decay reactions	3233
30.	B. Sagar Ref: 151	Analytic & Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	VADOSE (1982)	Steady or transient, two-dimensional, areal, cross-sectional or radial simulation of density-dependent transport of moisture, heat and mass in variably saturated, heterogeneous, anisotropic porous media.	convection conduction dispersion diffusion hysteresis adsorption decay reactions	3234
31.	B. Sagar	Analytic & Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	FLOTRA (1982)	Steady or transient, two-dimensional, areal, cross-sectional or radial simulation of density-dependent flow, heat and mass transport in variably saturated, anisotropic, heterogeneous deformable porous media.	convection conduction dispersion diffusion consolidation hysteresis adsorption decay reactions	3235
32.	G.T. Yeh D.S. Ward	Environmental Sciences Division Oak Ridge National Lab Oak Ridge, TN 37830	FEMWASTE/ FECWASTE (1981)	A two-dimensional finite-element model for transient simulation of areal or cross-sectional transport of dissolved constituents for a given velocity field in a anisotropic, heterogeneous porous medium.	capillarity convection dispersion diffusion adsorption decay	3371

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
33.	G.T. Yeh D.D. Huff Ref: 199	Environmental Sci. Div. Oak Ridge National Lab. Oak Ridge, TN 37830	FEMA (1985)	A two-dimensional finite-element model to simulate solute transport including radioactive decay, sorption, and biological and chemical degradation. This model solves only the solute transport equation and velocity field must be generated by a flow model.	dispersion diffusion adsorption decay advection	3376
34.	D.L. Deangelis G.T. Yeh D.D. Huff Ref: 34	Envionmental Sci. Div. Oak Ridge National Lab. Oak Ridge, TN 37830	FRACPORT (1984)	An integrated compartmental model for describing the transport of solute in three-dimensional fractured porous medium.	advection dispersion adsorption decay	3374
35.	J.C. Parker M. Th. van Genuchten Ref: 183	Dept. of Agronomy Virginia Polytechn. Inst. and State Univ. Blacksburg, VA 24061	CXTFIT (1984)	To determine values for one-dimensional analytical solute transport parameters, using a nonlinear least-squares inversion method.	dispersion diffusion decay zero-order production advection	3432
36.	H. Fluhler W.A. Jury Ref: 51	Swiss Federal Inst. of Research CH 8903 Brimensdorf Switzerland	PISTON (1983)	A finite-difference approach to simulate transport of reactive solute species through soil columns by mass flow (convective transport) including instantaneous equilibrium and rate-dependent solute exchange between liquid and solid phase.	adsorption ion exchange reactions	3450
37.	H. Fluhler W.A. Jury Ref: 51	Swiss Federal Inst. of Research CH 8903 Birmensdorf Switzerland	DISPEQ /DISPER (1983)	Finite-difference approach to simulate transport of reactive solute species through soil columns, including dispersion, instantaneous equilibrium adsorption (DISPEQ) and rate-dependent adsorption (DISPER).	dispersion adsorption ion exchange reactions	3451
38.	Walter G. Knisel Ref: 90	U.S. Dept. of Agriculture Agricultural Research Service Southeast Watershed Research Lab. P.O. Box 946 Tifton, GA 31793	CREAMS (1982)	CREAMS is a general watershed model designed to evaluate nonpoint source pollution from alternate management practices for field-size areas. It consists of three main components: hydrology, erosion/sedimentation, and chemistry.	precipitation evapotranspiration adsorption decay	3540

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
39.	N.W. Kline R.L. England R.C. Boca Ref: 34	Rockwell International Rockwell Hanford Operations P.O. Box 800 Richland, WA 99352	CHAINT (1985)	A general purpose two-dimensional, finite-element model for radionuclide transport in a fractured porous medium. CHAINT includes advection, dispersion, diffusion, retardation and chain-decay. It requires output of the finite-element flow model MAGNUM.2D as input.	diffusion adsorption decay advection buoyancy chain-decay (two daughters)	3791
40.	C.I. Voss Ref: 188	U.S. Geological Survey National Center 12201 Sunrise Valley Dr. Reston, VA 22092	SUTRA (1984)	A finite-element simulation model for two-dimensional, transient or steady-state, saturated-unsaturated, density-dependent ground water flow with transport of energy or chemically reactive single species solutes.	capillarity convection dispersion diffusion adsorption reactions	3830
41.	F.M. Lewis C.I. Voss J. Rubin Ref: 101	U.S. Geological Survey National Center 12201 Sunrise Valley Dr. Reston, VA 22092	SATRA-CHEM (1986)	A two-dimensional integrated-finite-difference model for flow and solute transport in saturated porous media. The model is a modification of SATRA, a simplified version of SUTRA. It incorporates aqueous equilibrium-controlled reactions, and either linear adsorption or binary ion exchange.	advection dispersion adsorption ion exchange complexation	3831
42.	R.T. Dillon R.M. Cranwell R.B. Lantz S.B. Pahwa M. Reeves Ref: 144	Natl. Energy Software Center Argonne Natl. Laboratory 9700 S. Cass Avenue Argonne, IL 60439	SWIFT (1981)	A three-dimensional finite-difference model for simulation of coupled, transient, density-dependent flow and transport of heat, brine, tracers or radionuclides in anisotropic, heterogeneous saturated porous media.	advection dispersion diffusion adsorption ion exchange decay chemical reactions	3840
43.	A.B. Gureghian Ref: 62	ONWI, Battelle Memorial Institute 505 King Avenue Columbus, OH 43201	TRIPM (1983)	A two-dimensional finite-element model for the simultaneous transport of water and reacting solutes through saturated and unsaturated porous media.	capillarity dispersion adsorption decay advection	4081
44.	B.J. Travis Ref: 170	Earth and Space Sciences Division Los Alamos National Lab. Los Alamos, NM 87545	TRACR3D (1984)	A three-dimensional finite-difference model of transient two-phase flow and multicomponent transport in deformable, heterogeneous, porous/fractured media.	capillarity dispersion diffusion adsorption decay advection	4270

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
45.	C.J. Emerson B. Thomas R.J. Luxmoore Ref: 44	Computer Sciences Oak Ridge National Lab. Oak Ridge, TN 37831	CADIL (1984)	CADIL simulates chemical transport through soils and the effect of soil temperature on chemical degradation.	diffusion adsorption deposition chemical degradation	4290
46.	I.L. Nwaogazie Ref: 125	I.L. Nwaogazie Dept. of Civil Eng. Univ. of Port Harcourt PMB 5323 Port Harcourt, Nigeria	SOTRAN (1988)	A finite-element solute transport model for two-dimensional unconfined aquifer systems, using linear or quadratic isoparametric quadrilateral elements	dispersion adsorption advection biodegradation radioactive decay	4320
47.	M.J. Martinez Ref: 106	Fluid Mechanics and Heat Transfer Division Sandia National Laboratories Albuquerque, NM 87185	FEMTRAN (1984)	A two-dimensional finite-element model to simulate cross-sectional radionuclide transport in saturated/unsaturated porous media. The model considers chain-decay of the radionuclides. It requires user-prescribed heads.	capillarity advection decay	4350
48.	A.J. Russo Ref: 149	Fluid Mechanics and Heat Transfer Division Sandia National Laboratories Albuquerque, NM 87185	IONMIG (1984)	A finite-difference model to calculate two-dimensional transport of decaying radionuclides through a saturated porous medium.	dispersion diffusion adsorption decay	4360
49.	R.M. Li Ref: 20	Simous, Li & Assoc., Inc. P.O. Box 1816 Ft. Collins, CO 80522	SBIR (1984)	A three-dimensional finite-difference model for simulation of flow and mass transport in a variably saturated porous medium.	capillarity convection dispersion	4391
50.	A.L. Baehr Ref: 7	U.S. Geological Survey National Center 12201 Sunrise Valley Dr. Reston, VA 22092	GASOLINE (1985)	A one-dimensional model to solve a system of equations defining the transport of an immiscible contaminant immobilized in the unsaturated zone, with or without biodegradation.	advection dispersion biodegradation immiscible flow	4420
51.	G.A. Cederberg R.L. Street J.O. Leckie Ref: 23	Los Alamos National Lab MS F665 Los Alamos, NM 87544	TRANQL (1985)	TRANQL is a finite-element, coupled geochemical/transport model for a multicomponent solution system with equilibrium interaction chemistry coupled with one-dimensional advective-dispersive transport.	convection dispersion adsorption ion exchange reactions	4450
52.	D.N. Contractor S.M.A. El Didy A.S. Ansary Ref: 25	Department of Civil and Mechanical Engineering University of Arizona Tucson, AZ 85721	MAQWQ (1986)	A finite-element model for simulation of transient nonconservative transport of contaminants in a multiple aquifer system, using velocities generated by the code MAQWF.	dispersion diffusion adsorption decay advection	4531

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
53.	C.M. King E.L. Wilhite R.W. Root Jr. D.J. Fauth K.R. Routt R.H. Emslie R.R. Beckmeyer Ref: 89	E.I. Dupont de Nemours and Corp. Savannah River Lab. Aiken, S.C.	DOSTOMAN (1985)	A finite-difference compartmental model for estimation of long-term dose to humans from buried waste.	diffusion adsorption ion exchange decay reactions advection	4540
54.	O.D. Nielsen P. Bo, L. Carlsen Ref: 119	Chemistry Dept. Riso National Laboratory P.O. Box 49 DK-4900, Denmark	COLUMN2 (1985)	One-dimensional simulation of solute transport in column experiments, using a finite-difference approach combined with the method of characteristics to solve the transient nonconservative transport equation.	dispersion adsorption ion exchange decay reactions advection hydrolysis complexation	4560
55.	K.L. Kipp Ref: 91	IGWMC Holcomb Research Institute 4600 Sunset Ave. Indianapolis, IN 46208	HST3D (1988)	A density-dependent, three-dimensional, finite-difference model for simulation of heat and solute transport.	advection dispersion diffusion retardation decay	4610
56.	A.B. Gureghian Ref: 63	Office of Crystalline Repository Development Battelle Memorial Institute 505 King Avenue Columbus, Ohio 43201	MASCOT (1986)	Analytical solutions for multidimensional transport of a four-member radionuclide decay chain in groundwater.	diffusion decay reactions advection dispersion	4620
57.	P.S. Huyakorn Ref: 74	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	FLAMINCO (1985)	A three-dimensional finite-element code for analyzing water flow and solute transport in saturated-unsaturated porous media.	evapotranspiration dispersion diffusion adsorption decay advection	4630
58.	P.S. Huyakorn Ref: 73	HydroGeoLogic, Inc. 503 Carlisle Dr., Suite 250 Herndon, VA 22070	VAM2D (1988)	A two-dimensional finite-element model to simulate flow and contaminant transport in variably saturated porous media. This code can perform simulations in an areal plane, a cross-section, or an axisymmetric configuration. It can also handle highly nonlinear soil moisture relations.	recharge infiltration evapotranspiration advection dispersion adsorption degradation	4690
59.	P.S. Huyakorn Ref: 76	HydroGeoLogic, Inc. 503 Carlisle Dr., Suite 250 Herndon, VA 22070	VAM3D (1988)	A three-dimensional finite-element model that simulates flow and contaminant transport in variably saturated porous media. It is capable of steady-state and transient simulations in an areal plane, a cross-section, an axisymmetric configuration, or as fully three-dimensional.	advection dispersion adsorption degradation	4691

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
60.	P.S. Huyakorn Ref: 77	HydroGeoLogic, Inc. 503 Carlisle Dr., Suite 250 Herndon, VA 22070	DSTRAM (1988)	A three-dimensional finite-element model that simulates density-dependent single-phase fluid flow and solute or energy transport in saturated porous media. This model can perform steady-state or transient simulations in a cross-section, an axisymmetric configuration, or a fully 3-D model, and it is designed specifically for situations where groundwater flow is influenced by variations in solute concentration or temperature.	infiltration aquitard leakage advection dispersion adsorption degradation conduction heat storage	4700
61.	R.F.Carsel C.N. Smith L.A. Mulkey J.D. Dean P. Jowise Ref: 22	Environmental Research Lab Office of Research and Development U.S. EPA Athens, GA 30613	PRZM (1984)	The Pesticide Root Zone Model simulates the vertical movement of pesticides in the unsaturated zone. The model consists of hydrologic and chemical transport components to simulate runoff, erosion, plant uptake, leaching, decay, foliar washoff, and volatilization.	runoff erosion plant uptake leaching decay foliar washoff volatilization	4720
62.	M. Bonazountas J.M. Wagner Ref: 14	Office of Toxic Substances U.S. EPA Washington, DC	SESOIL (1984)	A user-friendly model for long-term environmental pollutant fate simulations. SESOIL is designed to describe flow, sediment transport, pollutant transport and transformation, pollutant migration to groundwater, and soil quality.		4730
63.	P.K.M. van der Heijde Ref: 179	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	PLUME2D (1986)	An analytical solution to calculate concentration distribution in a homogeneous nonleaky, confined aquifer with uniform regional flow. The model uses the well function for solute convection and dispersion in a system with continuously injecting, fully penetrating wells.	convection dispersion retardation decay	6024
64.	M.Th. van Genuchten W.J. Alves Ref: 184	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	ONE-D (1985)	A package of five analytical solutions to the one-dimensional convection-dispersion equation with linear adsorption, zero-order production, and first-order decay.	convection dispersion adsorption decay	6220 6221 6222 6223 6224

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
65.	M.Th. van Genuchten Ref: 185	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	CFITIM (1985)	A program for estimation of non-equilibrium solute transport parameters from miscible displacement experiments.		6227
66.	I. Javandel L. Doughty C.F. Tsang Ref: 85	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	AGU-10 (1988)	A package of analytical and semi-analytical solutions for solute transport which includes one-and two-dimensional solutions (ODAST, TDAST), a semi-analytical solution for radial dispersion (LTIRD), and a streamline-tracking solution (RESSQ).	convection dispersion decay adsorption	6310 6311 6312 3940 3941
67.	W.C. Walton Ref: 190	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	WALTON 35 (1985)	A series of analytical and simple numerical models to analyze flow and solute and heat transport in confined, leaky confined, and water table aquifers with simple geometry.	convection dispersion stream depletion upconing conduction induced infiltration	6350
68.	M.S. Beljin Ref: 9	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	SOLUTE (1985)	A package of eight analytical models for solute transport. The models vary according to dimensional capabilities and boundary conditions.	convection dispersion adsorption decay	6380
69.	J. Bear A Verruijt Ref: 8	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	BEAVERSOFT (1987)	A package of analytical and numerical solutions for groundwater flow and solute transport. The package includes models for steady and unsteady two-dimensional flow in heterogeneous aquifers, for flow through dams, contaminant transport by advection and dispersion and for salt water intrusion.	convection, dispersion	6590
70.	J.P. Sauty W. Kinzelbach Ref: 152	IGWMC Holcomb Research Institute 4600 Sunset Avenue Indianapolis, IN 46208	CATTI (1988)	A program for the interpretation of tracer test data. CATTI computes breakthrough curves based on instantaneous or continuous injection of tracer into a homogeneous aquifer with either 1D-2D uniform flow or axisymmetric flow for one or two layers. The package includes a parameter optimization procedure.		6600
71.	P. Srinivasan J.W. Mercer Ref: 160	GeoTrans, Inc. 250 Exchange Place, Suite A Herndon, VA 22070	BIO-1D (1988)	A one-dimensional solute transport model which simulates aerobic and anaerobic degradation with or without adsorption for both substrate and oxygen.	convection adsorption biodegradation	6610

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
72.	D.L. Nofziger J.R. Williams T.E. Short Ref: 120	Robert S. Kerr Environmental Research Lab U.S. EPA Ada, OK 74820	RITZ (1988)	The Regulatory and Investigative Treatment Zone Model is an interactive model for simulation of the movement and fate of hazardous chemicals during land treatment of oily wastes.	volatilization degradation leaching	6620
73.	D.L. Nofziger P.S.C. Rao A.G. Hornsby Ref: 122	Institute of Food and Agricultural Sciences University of Florida Gainesville, FL 32611	CHEMRANK (1988)	A package which utilizes four schemes for screening of organic chemicals relative to their potential to leach into groundwater systems. The schemes are based on rates of chemical movement or relative rates of mobility and degradation of the chemicals within the vadose zone.	leaching degradation mobility	6640

APPENDIX C2 SOLUTE TRANSPORT MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
1.	P.S.C. Rao	NITROSIM	U	U	Y	Y	Y	U	Y	U	Y	Y	F	0280
2.	H.M. Selim J.M. Davidson	NMODEL	U	U	Y	Y	L	N	Y	Y	Y	L	F	0290
3.	G.F. Pinder	ISOQUAD 2	U	G	Y	Y	N	Y	Y	U	Y	L	U	0511
4.	P.S. Huyakorn	TRAFRAP-WT	N	N	Y	Y	N	Y	Y	Y	Y	L	M	0581
5.	P.S. Huyakorn	GREASE 2	N	N	Y	Y	N	Y	U	U	Y	L	F	0582
6.	P.S. Huyakorn	SATURN 2	N	N	Y	Y	N	Y	Y	U	Y	L	F	0583
7.	P.S. Huyakorn	SEFTRAN	D	G	Y	Y	N	Y	Y	Y	Y	Y	M	0588
8.	T.R. Knowles	GWSIM-II	U	G	Y	Y	Y	N	U	U	Y	L	F	0680
9.	INTERA Env. Cons., Inc.	SWIPR	U	U	Y	Y	L	Y	Y	U	Y	Y	F	0693
10.	L.F. Konikow J.O. Bredehoeft	USGS-2D-TRANSPORT/MOC	Y	N	Y	Y	N	Y	Y	Y	Y	Y	M	0740
11.	S.P. Garabedian L.F. Konikow	FRONTTRACK	N	G	Y	Y	N	Y	Y	U	Y	U	F	0741
12.	S.W. Ahlstrom	MMT-DRPW	Y	Y	Y	Y	N	Y	U	Y	Y	U	F	0780
13.	F.E. Kaszeta, et al.	MMT-1D	Y	Y	Y	Y	Y	U	U	U	Y	L	U	0781
14.	V. Guvanasen	MOTIF	U	U	Y	Y	N	Y	Y	U	Y	L	M	0953
15.	I. Miller	Golder Groundwater Computer Package	D	D	Y	Y	N	Y	U	U	Y	L	F	1010
16.	S.K. Gupta, et al.	CFEST	Y	Y	Y	Y	Y	Y	Y	Y	Y	L	M	2070
17.	H.C. Burkholder, et al.	GETOUT	U	U	Y	Y	L	Y	Y	U	Y	U	M	2080
18.	R.W. Nelson	PATHS	Y	Y	Y	Y	Y	Y	Y	Y	Y	L	M	2120

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APPENDIX C2 SOLUTE TRANSPORT MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
19.	R.D. Schmidt	ISL-50	U	U	Y	Y	L	N	Y	U	Y	L	F	2560
20.	T.A. Prickett T.G. Naymit C.G. Lonnquist	RANDOM WALK	Y	G	Y	Y	N	L	Y	Y	Y	Y	M	2690
21.	B. Ross C.M. Koplik	WASTE	U	U	Y	Y	Y	Y	Y	U	Y	L	F	2810
22.	L.A. Davis G. Segol	GS2	U	U	Y	Y	Y	Y	Y	Y	Y	U	F	2891
23.	L.A. Davis G. Segol	GS3	U	U	Y	Y	Y	Y	Y	Y	Y	U	F	2892
24.	J.W. Wesseling	GROWKWA	U	U	Y	Y	Y	Y	Y	U	U	U	F	2982
25.	J. Noorishad	ROCMAS-HS	U	U	Y	Y	U	N	Y	U	Y	L	F	3081
26.	J.W. Warner	RESTOR	U	U	Y	Y	U	Y	Y	U	Y	L	F	3100
27.	S. Haji-Djafari T.C. Wells	GEOFLOW	U	U	Y	Y	Y	Y	Y	U	Y	L	F	3220
28.	B. Sagar	FRACFLOW	Y	Y	Y	Y	N	Y	U	U	Y	U	F	3232
29.	A.K. Runchal	PORFLOW	N	Y	Y	Y	N	Y	Y	Y	Y	Y	M	3233
30.	B. Sagar	VADOSE	U	U	Y	Y	N	Y	U	U	Y	U	F	3234
31.	B. Sagar	FLOTRA	U	U	Y	Y	N	Y	U	U	Y	L	F	3235
32.	G.T. Yeh D.S. Ward	FEMWASTE/ FECWASTE	N	N	Y	Y	Y	Y	Y	Y	Y	L	M	3371
33.	G.T. Yeh D.D. Huff	FEMA	N	G	Y	Y	N	Y	Y	U	Y	L	F	3376
34.	D.L. Deangelis, et al.	FRACPORT	N	N	Y	Y	U	N	Y	U	Y	U	F	3374
35.	J.C. Parker M.Th. van Genuchten	CXTFIT	U	U	Y	Y	N	Y	U	U	Y	L	F	3432
36.	H. Fluhler W.A. Jury	PISTON	N	N	Y	Y	Y	Y	Y	Y	Y	U	F	3450

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APPENDIX C2 SOLUTE TRANSPORT MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
37.	H. Fluhler W.A. Jury	DISPEQ/ DISPER	N	N	Y	Y	Y	Y	Y	Y	Y	U	F	3451
38.	W. G. Knisel	CREAMS	U	U	Y	Y	N	Y	Y	Y	Y	Y	M	3540
39.	N.W. Kline, et al.	CHAINT	N	N	Y	Y	L	Y	U	U	Y	L	F	3791
40.	C.I. Voss	SUTRA	Y	Y	Y	Y	N	Y	Y	Y	Y	Y	M	3830
41.	F.M. Lewis, et al.	SATRA- CHEM	N	N	Y	Y	U	L	U	U	Y	U	U	3831
42.	R.T. Dillon, et al.	SWIFT	N	G	Y	Y	N	Y	Y	Y	Y	Y	M	3840
43.	A.B. Gureghian	TRIPM	U	U	Y	Y	Y	Y	Y	U	Y	U	F	4081
44.	B.J. Travis	TRACR3D	N	Y	Y	Y	Y	Y	U	U	Y	U	F	4270
45.	C.J. Emerson, et al.	CADIL	U	U	Y	Y	Y	Y	Y	Y	Y	L	F	4290
46.	I.L. Nwaogazie	SOTRAN	U	U	Y	Y	U	N	Y	U	Y	U	F	4320
47.	M.J. Martinez	FEMTRAN	U	U	Y	Y	L	Y	Y	U	Y	L	F	4350
48.	A.J. Russo	IDNMIG	U	U	Y	Y	L	Y	U	U	Y	L	U	4360
49.	R.M. Li	SBIR	U	U	Y	Y	Y	Y	Y	U	Y	U	F	4391
50.	A.L. Baehr	GASOLINE	U	U	Y	Y	Y	N	Y	U	Y	U	F	4420
51.	G.A. Cederberg, et al.	TRANQL	U	U	U	U	L	L	Y	Y	Y	U	U	4450
52.	D.N. Contractor, et al.	MAQWQ	U	U	Y	U	L	U	U	U	Y	U	U	4531
53.	C.M. King, et al.	DOSTOMAN	U	U	Y	Y	Y	Y	Y	U	Y	L	F	4540
54.	O.J. Nielsen, et al.	COLUMN2	U	U	Y	U	U	U	U	U	Y	U	U	4560
55.	K.L. Kipp	HST3D	N	N	Y	Y	N	Y	Y	Y	Y	L	F	4610
56.	A.B. Gureghian	MASCOT	U	U	Y	Y	L	N	U	U	Y	U	U	4620
57.	P.S. Huyakorn	FLAMINCO	N	N	Y	Y	Y	Y	Y	Y	Y	Y	F	4630
58.	P.S. Huyakorn	VAM2D	N	N	Y	Y	N	Y	Y	U	Y	L	F	4690

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APPENDIX C2 SOLUTE TRANSPORT MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
59.	P.S. Huyakorn	VAM3D	N	N	Y	Y	N	Y	Y	U	Y	L	F	4691
60.	P.S. Huyakorn	DSTRAM	N	N	Y	Y	N	Y	Y	U	Y	L	F	4700
61.	R.F. Carsel, et al.	PRZM	D	N	Y	Y	U	L	U	U	Y	L	F	4720
62.	M. Bonazantas J.M. Wagner	SESOIL	D	U	Y	Y	U	N	U	U	U	U	F	4730
63.	P.K.M. van der Heijde	PLUME2D	D	N	Y	Y	L	Y	Y	N	Y	L	M	6024
64.	M.Th. van Genuchten W.J. Alves	ONE-D	D	N	Y	Y	N	L	Y	N	Y	U	F	6220- 6224
65.	M.Th. van Genuchten	DFITIM	N	N	Y	Y	N	L	U	U	Y	L	F	6227
66.	I. Javandel, et al.	AGU-10	N	Y	Y	Y	L	Y	Y	N	Y	L	M	6310 6311 6312 3940 3941
67.	W.C. Walton	WALTON 35	D	N	Y	Y	L	L	Y	U	Y	L	M	6350
68.	M.S. Beljin	SOLUTE	D	D	Y	Y	L	Y	Y	N	Y	L	M	6380
69.	J. Bear A. Verruijt	BEAVER-SOFT	D	D	Y	N	L	L	Y	U	Y	L	M	6590
70.	J.P. Sauty W. Kinzelbach	CATTI	D	D	Y	Y	L	L	U	U	Y	U	F	6600
71.	P. Srinivasan J.W. Mercer	BIO-1D	D	D	Y	Y	L	Y	U	U	Y	L	F	6610
72.	D.L. Nofziger, et al.	RITZ	D	N	Y	Y	U	L	U	U	Y	L	F	6620
73.	D.L. Nofziger, et al.	CHEMRANK	D	U	Y	Y	U	L	U	U	U	U	F	6640

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APPENDIX D1 HEAT TRANSPORT MODELS: SUMMARY LISTING

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	M.J. Lippman T.N. Narasimhan D.C. Mangold G.S. Bodvarsson Ref: 104	Nat'l Energy Software Center Argonne Nat'l Lab. 9700 S. Cass Ave. Argonne, IL 60439	PT/CCC (1981)	Model uses integrated-finite-difference method to calculate steady and unsteady temperature and pressure distributions, and vertical compaction in multidimensional heterogeneous systems with complex geometry and a single phase, non-isothermal liquid.	Heat convection conduction, consolidation expansion	0100
2.	M.L. Sorey M.J. Lippman Ref: 39	Nat'l Energy Software Center Argonne Nat'l Lab. 9700 S. Cass Ave. Argonne, IL 60439	SCHAFF (1974)	A three-dimensional finite-difference model to simulate unsteady heat and fluid flow in slightly compressible porous media.	Heat convection conduction	0160
3.	G.F. Pinder P.E. Kinnmark C.I. Voss Ref: 134	Dept. of Civil Engineering School of Engineering & Applied Science Princeton Univ. Princeton, NJ 05844	GAFETTA (1980)	Prediction of heads and temperatures by finite-element simulation of two-dimensional, horizontal flow and heat transport (steady-state or transient) in isotropic, heterogeneous aquifers.	Heat convection conduction dispersion	0513
4.	P.S. Huyakorn	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	SEFTRAN (1985)	A two-dimensional finite-element model for simulation of transient flow and transport of heat or solutes in anisotropic, heterogeneous porous media.	advection dispersion diffusion adsorption decay	0588
5.	P.S. Huyakorn Ref: 70	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	GREASE2 (1982)	The finite-element model simulates heat and/or solute transport in fractured porous media. The flow field is multi-dimensional, density-dependent, transient or steady-state in anisotropic heterogeneous, confined, or unconfined aquifers.	Heat convection conduction dispersion solute convection, diffusion adsorption	0582
6.	P.S. Huyakorn Ref: 78	IGWMC Holcomb Research Institute 4600 Sunset Ave. Indianapolis, IN 46208	TRAFRAP-WT (1987)	Two-dimensional finite-element model to simulate fluid flow and transport of radionuclides in fractured porous media.	Heat convection conduction in fluid dispersion	0589
7.	J.E. Reed Ref: 143	M.S. Bedinger U.S. Geological Survey Box 25046, MS 417 Federal Center Denver, CO 80225	HOTWTR (1985)	A finite-difference model to simulate steady-state coupled fluid and heat flow in an isotropic heterogeneous aquifer system with uniform thermal properties and viscosity-dependent hydraulic conductivity.	Heat convection and conduction coupled with flow	0612

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
8.	INTERA, Inc. Ref: 84	INTERA Technologies, Inc. 6850 Austin Ctr. Blvd. Suite 300 Austin, TX 78731	SWENT (1983)	Multidimensional finite-difference model to simulate fluid flow, heat, and radioactive contaminant transport in heterogeneous porous media.	Heat convection conduction dispersion vertical heat loss	0692
9.	K.L. Kipp Ref: 91	K. Kipp U.S. Geological Survey Box 25046, Mail Stop 411 Denver Federal Center Lakewood, CO 80225	HST3D (1988)	A finite-difference model to simulate non-steady three-dimensional groundwater flow, heat, and contaminant transport in a heterogeneous aquifer.	Heat convection, conduction, and dispersion; pressure effects on enthalpy; solute convection, diffusion, dispersion, adsorption/ desorption, and decay	4610
10.	C.R. Faust J.W. Mercer Ref: 48	ONWI Battelle Project Mgmnt. Division 505 King Avenue Columbus, OH 43201	GEOTHER (1983)	Finite-difference simulation of transient, three-dimensional, single and two-phase, heat transport in anisotropic, heterogeneous, porous media.	Heat convection, conduction, dispersion, and diffusion; condensation; change of phase	0730
11.	S.W. Ahlstrom H.P. Foote R.J. Serne Ref: 2	Battelle Pacific NW Labs P.O. Box 999 Richland, WA 99352	MMT-DPRW (1976)	Model using discrete parcel random walk method to predict transient, three-dimensional movement of radionuclides, heat and other contaminants in saturated/unsaturated aquifer systems.	advection dispersion diffusion adsorption decay chemical reactions ion exchange dissolution precipitation	0780
12.	F.E. Kaszeta C.S. Simmons C.R. Cole Ref: 192	Battelle Pacific NW Labs P.O. Box 999 Richland, WA 99352	MMT-1D (1980)	A discrete parcel random walk model to simulate transient, one-dimensional movement of radionuclides, heat and other contaminants in saturated/unsaturated aquifer systems (1-D version of MMT-DPRW).	advection dispersion diffusion sorption decay chemical reactions	0781
13.	V. Guvanasen Ref: 24	Applied Geoscience Branch Whiteshell Nuclear Res. Atomic Energy of Canada Pinawa, Manitoba Canada ROE 1LO	MOTIF (1986)	A finite-element model for one-, two-, and three-dimensional saturated/unsaturated groundwater flow, heat transport, and solute transport in fractured porous media. The model considers single-species radionuclide transport and solute diffusion from fracture to rock matrix.	Capillarity; heat convection; solute convection, dispersion, diffusion, adsorption, and decay	0953

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
14.	J.F. Pickens G.E. Grisak Ref: 131	INTERA Technologies Inc. 6850 Austin Ctr. Blvd. Suite 300 Austin, TX 78731	SHALT (1980)	The model simulates heat and solute transport in a fractured, saturated or unsaturated, two-dimensional aquifer. The finite-element technique is used in the solution of the equation describing density-dependent, compressible fluid, steady-state or transient situations.	Heat convection, conduction, and dispersion; solute convection, dispersion, adsorption, radioactive decay, and chemical reactions	2034
15.	S.K. Gupta C.R. Cole C.T. Kincaid A.M. Monti Ref: 59	Water and Land Resources Division Battelle Pacific NW Lab P.O. Box 999 Richland, WA 99352	CFEST (1987)	Two- or three-dimensional finite-element simulation of steady-state or transient flow, energy and solute transport in anisotropic heterogeneous multilayered aquifers.	Heat convection, conduction, solute convection, dispersion, and diffusion	2070
16.	K. Pruess R.C. Schroeder Ref: 140	Nat'l Energy Software Center Argonne Nat'l Lab 9700 S. Cass Ave. Argonne, IL 60439	SHAFT79 (1980)	Transient simulation of simultaneous three-dimensional heat and fluid transport in porous media using finite-difference and integrated-finite-difference methods.	condensation; heat convection, and conduction; change of phase	2580
17.	K. Pruess Ref: 141	Mail Stop 50E Lawrence Berkeley Lab Berkeley, CA 94720	MULKOM (1985)	An integrated-finite-difference model to simulate heat and multiphase fluid flow in multidimensional fractured porous media; the method adopted is a generalization of the double-porosity approach.	Heat convection and conduction; Fluid (water and gas) transport; change of phase; solute convection; dissolution and precipitation, transport of dissolved solids	2581
18.	D.K. Gartling Ref: 54	Sandia Nat'l Labs Division 5511 Albuquerque, NM 87185	MARIAH (1980)	A finite-element model to simulate unsteady two-dimensional vertical flow in anisotropic heterogenous porous media with heat transfer.	Heat convection, conduction, and dispersion	2620

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
19.	J.W. Pritchett Ref: 139	Systems, Science and Software P.O. Box 1620 La Jolla, CA 92038	MUSHRM (1980)	Multispecies hydrothermal reservoir model to simulate unsteady multiphase fluid and heat flow in multidimensional geometries by means of finite-difference method.	Heat convection, and conduction; degassing, consolidation; expansion; change of phase (flow is coupled)	2760
20.	J.W. Pritchett Ref: 139	Systems, Science and Software P.O. Box 1620 La Jolla, CA 92038	CHARGR (1980)	Hydrothermal reservoir model using finite-difference method to predict pressures and temperatures in anisotropic, heterogeneous confined aquifers with matrix deformation; simulation of three-dimensional transient multiphase flow of a compressible fluid with dissolved incondensible gases and heat transport.	Heat convection and conduction; change of phase (flow is coupled)	2761
21.	A.K. Runchal J. Treger G. Segal Ref: 147	Dames and Moore Advanced Technology Group 1100 Glendon Ave., Suite 1000 Los Angeles, CA 90024	EP21-GWTHERM (1979)	An integrated-finite-difference model to simulate fluid flow and heat and solute transport in an anisotropic, heterogeneous, water-table aquifer. The flow field is two-dimensional, density-dependent and steady-state or transient.	Heat convection and dispersion; solute convection, dispersion, diffusion, retardation and radioactive decay	2830
22.	C.B. Andrews Ref: 6	Woodward-Clyde Cnslt. Three Embarcadero Center, Suite 700 San Francisco, CA 94111	UWIS-2D-TRANSPORT (1980)	Model using finite-element method to simulate two-dimensional, areal or cross-sectional, steady or transient, single-phase, heat or conservative solute transport in a confined or phreatic, anisotropic, heterogeneous aquifer.	Heat convection, conduction, and dispersion; solute convection, dispersion, diffusion, adsorption, and absorption	2860
23.	W.R. Walker J.D. Sabey Ref: 189	Water Resources Research Center Virginia Polytechnic Institute 617 North Main St. Blacksburg, VA 24060	TRANS (1981)	The finite-element model predicts heads, flow rates, moisture contents and temperatures by simulating two-dimensional horizontal or vertical, transient flow and heat transport in anisotropic, heterogeneous, variably saturated soil.	Heat convection, conduction, and dispersion (coupled with flow)	2950

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
24.	B. Sagar	Analytic & Computational Research, Inc. 3016 Inglewood Blvd. Los Angeles, CA 90066	VADOSE (1982)	Steady or transient, two-dimensional, areal, cross-sectional or radial simulation of density-dependent transport of moisture, heat and mass in variably saturated, heterogeneous, anisotropic porous media.	convection conduction dispersion diffusion hysteresis adsorption decay reactions	3234
25.	B. Sagar	Analytic & Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	FLOTRA (1982)	Steady or transient, two-dimensional, areal, cross-sectional or radial simulation of density-dependent flow, heat and mass transport in variably saturated, anisotropic, heterogeneous deformable porous media.	convection conduction dispersion diffusion consolidation hysteresis adsorption decay reactions	3435
26.	A.K. Runchal	Analytic & Computational Res. Inc. 3106 Inglewood Blvd. Los Angeles, CA 90060	PORFREEZE (1981)	The model simulates density-dependent flow and heat transport in two-dimensional freezing-soil domains. The coupled equations represent saturated steady-state or transient conditions and are solved using the finite-difference approach. The system modeled is anisotropic and heterogeneous.	Heat convection and conduction	3236
27.	G.T. Yeh R.J. Luxmoore	Environmental Sci. Div. Oak Ridge National Lab Oak Ridge, TN 37830	MATTUM (1983)	A three-dimensional model for simulating moisture and heat transport in unsaturated porous media. The model solves both the flow and heat equation using the integrated compartment method.	Capillarity heat convection, conduction, and latent transfer due to evaporation	3375
28.	P.C.D. Milly Ref: 110	Massachusetts Inst. of Technology Dept. of Civil Eng. Cambridge, MA 02139	SPLASHWATR (1983)	One-dimensional, vertical finite-element simulation of steady or transient saturated/ unsaturated flow and heat transport in isotropic, heterogeneous soils to predict heads, flow rates and temperatures.	Heat convection, conduction, and dispersion	3590

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
29.	N.W. Kline A.K. Runchal R.G. Baca Ref: 93	Rockwell Hanford Operations Energy Systems Group Rockwell International P.O. Box 800 Richland, WA 99352	PORFLOW (1983)	An integrated-finite-difference model for simulating transient, two-dimensional or axisymmetric transfer and transport of radionuclides in layered geologic systems.	Heat convection and conduction; solute dispersion, diffusion, adsorption, decay, and retardation	3790
30.	C.I. Voss Ref: 188	U.S. Geological Survey National Center 12201 Sunrise Valley Dr. Reston, VA 22092	SUTRA (1985)	A finite-element simulation model for two-dimensional, transient or steady-state, saturated-unsaturated, density-dependent groundwater flow. Transport of either energy or dissolved substances is also included.	Capillarity; heat convection, dispersion, and conduction; solute convection, dispersion, diffusion, adsorption, and reactions (flow is coupled with either heat or solute transport)	3830
31.	R.T. Dillon R.M. Cranwell R.B. Lantz S.B. Pahwa M. Reeves Ref: 144	National Energy Software Center Argonne National Lab. 9700 S. Cass Ave. Argonne, IL 60439	SWIFT (1981)	A three-dimensional finite-difference model for simulating coupled, transient, density-dependent flow and transport of heat, brine, tracers or radionuclides in anisotropic, heterogeneous confined aquifers.	Heat convection and conduction; solute convection, dispersion, diffusion, adsorption, ion exchange, and decay, reaction, and buoyancy; salt dissolution	3840
32.	A.S. Bodvarsson Ref: 13	Earth Sciences Div. Lawrence Berkeley Lab. University of California Berkeley, CA 94720	PT (1983)	Model using finite-difference and integrated-finite-difference methods to simulate transient three-dimensional fluid flow and heat transport and one-dimensional subsidence in isotropic, heterogeneous, porous media.	Heat convection, and conduction; consolidation; expansion	3890
33.	E.K. Grubaugh D.L. Reddell Ref: 58	E.K. Grubaugh Texas Water Res. Inst. Texas A&M Univ. College Station, TX 77843	TEXASHEAT (1980)	A three-dimensional, transient finite-element model for solution of simultaneous flow and heat transport through anisotropic, heterogeneous porous media.	Heat convection and conduction; coupled with flow	3970

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
34.	A.L. Edwards A. Rasmuson I. Neretnicks T.N. Narasimhan Ref: 38	Dept. of Chemical Eng. Royal Inst. of Tech. S-100 44 Stockholm, Sweden	TRUMP (1980)	A multidimensional model, based on the integrated-finite-difference method, to simulate steady-state or transient flow and heat or solute transport in fractured rock.	Heat convection, dispersion, and conduction; solute dispersion, convection, diffusion, and decay (flow is coupled with either heat or solute transport)	4030
35.	C.A. Anderson Ref: 5	Los Alamos Nat'l Lab. Los Alamos, NM 87545	SANGRE (1986)	Two-dimensional finite-element program to simulate groundwater flow, heat transport and faulting in highly deformable porous aquifers.	Heat convection, conduction	4600
36.	R.L. England M.W. Kline K.J. Ebblad R.G. Baca Ref: 45	Rockwell Hanford Operations P.O. Box 800 Richland, WA 99352	MAGNUM-2D (1985)	Two-dimensional model, based on finite-element method, to simulate groundwater flow and heat transfer in fractured porous medium.	Heat convection, conduction, and dispersion	4590

APPENDIX D2 HEAT TRANSPORT MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
1	M.J. Lippman, et al.	PT/CCC	U	U	Y	Y	N	Y	Y	Y	Y	L	M	0100
2	M.L. Sorey M.J. Lippman	SCHAFF	U	U	Y	Y	N	Y	Y	Y	Y	L	F	0160
3	G.F. Pinder, et al.	GAFETTA	N	N	Y	Y	N	Y	Y	U	Y	L	F	0513
4	P.S. Huyakorn	SEFTRAN	D	G	Y	Y	N	Y	Y	Y	Y	Y	M	0588
5	P.S. Huyakorn	GREASE2	N	N	Y	Y	N	Y	Y	U	Y	L	F	0582
6	P.S. Huyakorn	TRAFRAP-WT	U	U	Y	Y	N	Y	Y	Y	Y	L	M	0589
7	J.E. Reed	HOTWTR	U	U	Y	Y	N	U	Y	U	Y	U	U	0612
8	INTERA, Inc.	SWENT	U	U	Y	Y	U	Y	Y	Y	Y	L	M	0692
9	K. Kipp	HST3D	N	D	Y	Y	N	Y	Y	Y	Y	L	F	4610
10	C.R. Faust J.W. Mercer	GEOTHER	U	U	Y	Y	N	Y	Y	Y	Y	L	F	0730
11	S.W. Ahlstrom, et al.	MMT-DPRW	Y	Y	Y	Y	N	Y	Y	Y	Y	U	F	0780
12	F.E. Kaszeta, et al.	MMT-1D	Y	Y	Y	Y	N	Y	Y	U	Y	U	U	0781
13	V. Guvanasen	MOTIF	U	U	Y	Y	N	N	Y	U	Y	U	M	0953
14	J.F. Pickens G.E. Grisak	SHALT	U	U	Y	Y	N	Y	Y	U	Y	L	M	2034
15	S.K. Gupta, et al.	CFEST	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	M	2070
16	K. Pruess R.C. Schroeder	SHAFT79	Y	U	Y	Y	N	Y	Y	U	Y	L	M	2580
17	K. Pruess	MULKOM	U	U	Y	Y	N	Y	Y	U	Y	L	M	2581
18	D.K. Gartling	MARIAH	U	U	Y	Y	N	U	Y	U	Y	U	F	2620
19	J.W. Pritchett	MUSHRM	U	U	Y	Y	N	Y	Y	U	Y	L	F	2760
20	J.W. Pritchett	CHARGR	U	U	Y	Y	N	Y	Y	U	Y	U	F	2761

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
21	A.K. Runchal, et al.	EP21-GWTHERM	U	U	Y	Y	N	Y	U	U	Y	L	F	2830
22	C.B Andrews	UWIS-2D-TRANSPORT	U	U	Y	Y	N	Y	Y	U	Y	L	F	2860
23	W.R. Walker J.D. Sabey	TRANS	U	U	Y	Y	N	U	U	U	Y	U	F	2950
24	B. Sagar	VADOSE	U	U	Y	Y	N	Y	U	U	Y	U	F	3234
25	B. Sagar	FLOTRA	U	U	Y	Y	N	Y	U	U	Y	L	F	3234
26	A.K. Runchal	PORFREEZE	U	U	Y	Y	N	Y	Y	U	Y	L	F	3236
27	G.T. Yeh R.J. Luxmoore	MATTUM	U	U	Y	U	N	Y	U	U	Y	U	F	3375
28	P.C.D. Milly	SPLASHWATR	U	U	Y	Y	N	U	U	U	Y	U	F	3590
29	N.W. Kline, et al.	PORFLOW	N	Y	Y	Y	N	Y	Y	Y	Y	L	M	3790
30	C.I. Voss	SUTRA	Y	Y	Y	Y	N	Y	Y	Y	Y	L	M	3830
31	R.T. Dillon, et al.	SWIFT	N	G	Y	Y	N	Y	Y	Y	Y	L	M	3840
32	A.S. Bodvarsson	PT	U	U	Y	Y	N	Y	Y	Y	Y	L	M	3890
33	E.K. Grubaugh D.L. Reddell	TEXASHEAT	U	U	Y	Y	U	U	U	U	Y	U	F	3970
34	A.L. Edwards, et al.	TRUMP	N	N	Y	Y	U	N	Y	Y	Y	L	F	4030
35	C.A. Anderson	SANGRE	N	N	Y	Y	U	U	U	U	U	U	U	4600
36	R.L. England, et al.	MAGNUM-2D	Y	Y	Y	Y	N	Y	Y	U	Y	U	U	4590

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

APPENDIX E1 HYDROCHEMICAL MODELS: SUMMARY LISTING

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	D.L. Parkhurst L.N. Plummer D.C. Thorstenson Ref: 128	L.N. Plummer U.S. Geological Survey Water Resources Division 12201 Sunrise Valley Drive Reston, VA 22092	BALANCE (1982)	Using the chemical compositions of water samples from two points along a flow path and a set of mineral phases hypothesized to be the reactive constituents in the system, the program calculates the mass transfer necessary to account for the observed changes in composition between the two water samples.	mass balance on elements mixing end-member waters redox reactions isotope balance no thermodynamic constraints on the reactions	3400
2.	T.J. Wolery	T.J. Wolery Lawrence Livermore National Laboratory P.O. Box 808, L-204 Livermore, CA 94550	EQ3NR/6 (1983)	EQ3NR is a geochemical aqueous speciation/solubility program that can be used alone or in conjunction with EQ6, which performs reaction-path calculations. Accomodates up to 40 elements, 300 aqueous species, 15 gases, and 275 minerals.	redox reactions need not be at equilibrium	
3.	J.R. Morrey D.W. Shannon	Vasel W. Roberts Electric Power Research Institute 3412 Hillview Avenue Palo Alto, CA 94304	EQUILIB (1978)	Models chemical equilibria in geothermal brines at various elevated temperatures. Contains 26 elements, 200 aqueous species, 7 gases, and 186 minerals.	redox reactions	
4.	G. Sposito S.V. Mattigod	G. Sposito Department of Soil and Environmental Sciences University of California Riverside, CA 92521	GEOCHEM (1980)	A program for predicting the equilibrium distribution of chemical species in soil solution and other natural water systems. Includes 45 elements, 1853 aqueous species, 42 organic ligands, 3 gases, and 250 minerals and solids.	mass balance for each species redox reactions cation adsorption and exchange	
5.	J.C. Westall J.L. Zachary F.M.M. Morel	F.M.M. Morel Dept. of Civil Engineering Massachusetss Institute of Technology Cambridge, MA 02139	MINEQL2 (1980)	A program for the calculation of chemical equilibria in aqueous systems.	mass balance redox reactions surface adsorption	
6.	A.R. Felmy D.C. Girvin E.A. Jenne	David Disney ADP Section Environmental Research Lab. U.S. Environmental Protection Agency College Station Road Athens, GA 30613	MINTEQ (1987)	A program for calculating geochemical equilibria, containing the WATEQ3 database. Includes 31 elements, 373 aqueous species, 3 gases, and 328 solids.	mass balance for each component redox reactions ion exchange six surface complexation models	
7.	D.L. Parkhurst D.C. Thorstenson L.N. Plummer Ref: 127	L.N. Plummer U.S. Geological Survey Water Resources Division 12201 Sunrise Valley Drive Reston, VA 22092	PHREEQE (1980)	An equilibrium model that can calculate mass transfer as a function of stepwise temperature change or dissolution. Includes 19 elements, 120 aqueous species, 3 gases, and 21 minerals.	mass balance redox reactions for 3 elements ion exchange	2610

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
8.	G. Pickrell D.D. Jackson	D.D. Jackson Lawrence Livermore National Laboratory P.O. Box 808, L-329 Livermore, CA 94550	PROTOCOL (1984)	A coupled kinetic/equilibrium program for calculating dissolution reactions of inorganic solids in aqueous solution, with specific application to corrosion of vitrified nuclear waste by groundwater. Incorporates equilibrium routines from MINEQL.	kinetic submodels -empirical -dissolution of silica -surface coverage	
9.	S.E. Ingle M.D. Schuldt D.W. Schults	D.W. Schults Hatfield Marine Sci. Cntr. U.S. Environmental Protection Agency Newport, OR 97365	REDEQL.EPA (1978)	A program to compute aqueous equilibria for up to 20 metals and 30 ligands in a system. Includes 46 elements, 94 aqueous species, 2 gases, and 13 minerals/solids.	mass balance redox reactions complexation	
10.	D.K. Harriss S.E. Ingle D.K. Taylor V.R. Magnuson	V.R. Magnuson Department of Chemistry University of Minnesota Duluth, MN 55812	REDEQL-UMD (1984)	A program to compute equilibrium distributions of species concentrations in aqueous systems. Standard version includes 53 elements, 109 aqueous species, 2 gases, and 27 mixed solids	redox reactions surface complexation adsorption model	
11.	Y.K. Kharaka I. Barnes	Y.K. Kharaka U.S. Geological Survey, MS/427 345 Middlefield Road Menlo Park, CA 94025	SOLMNEQ (1973)	A program for computing the equilibrium distribution of species in aqueous solution. Includes 26 elements, 162 aqueous species, and 158 minerals.	mass balance of each element redox reaction	
12.	B.W. Goodwin M. Munday	B.W. Goodwin Atomic Energy of Canada Ltd. Whiteshell Nuclear Research Establishment Pinawa, Manitoba ROE 1LO Canada	SOLMNQ (1983)	An interactive chemical speciation program that calculates equilibrium distributions for inorganic aqueous species often found in groundwater, a FORTRAN version of SOLMNEQ. Includes 28 elements, 239 aqueous species, and 181 solids.	mass balance of each element aqueous species of uranium and plutonium added redox reactions	
13.	J.W. Ball E.A. Jenne D.K. Nordstrom	J.W. Ball U.S. Geological Survey, MS/21 345 Middlefield Road Menlo Park, CA 94025	WATEQ2 (1980)	A chemical equilibrium model for calculating aqueous speciation of major and minor elements among naturally occurring ligands.	mass balance redox reactions	
14.	J.W. Ball E.A. Jenne M.W. Cantrell	J.W. Ball U.S. Geological Survey MS/21 345 Middlefield Road Menlo Park, CA 94025	WATEQ3 (1981)	The WATEQ2 model with the addition of uranium species.	mass balance redox reactions	

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
15.	L.N. Plummer B.F. Jones A.H. Truesdell	L.N. Plummer U.S. Geological Survey Water Resources Division 12201 Sunrise Valley Drive Reston, VA 22092	WATEQF (1984)	A program to model the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. A FORTRAN version of the original WATEQ (1973) in PL/1.	mass balance redox reactions	

APPENDIX E2 HYDROCHEMICAL MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
1.	D.L. Parkhurst, et al.	BALANCE	N	N	Y	Y	N	Y	Y	Y	U	U	M	3400
2.	T.J. Wolery	EQ3NR/6	N	N	Y	Y	U	Y	U	U	U	L	F	--
3.	J.R. Morrey D.W. Shannon	EQUILIB	U	U	Y	U	L	L	U	U	U	U	F	--
4.	G. Sposito S.V. Mattigod	GEOCHEM	U	N	Y	Y	L	L	U	U	U	U	F	--
5.	J.C. Westall, et al.	MINEQL2	N	N	Y	Y	N	L	U	U	U	L	M	--
6.	A.R. Felmy, et al.	MINTEQ	U	U	Y	Y	L	L	U	U	U	U	M	--
7.	D.L. Parkhurst, et al.	PHREEQE	Y	N	Y	Y	N	Y	Y	Y	U	U	M	2610
8.	G. Pickrell D.D. Jackson	PROTOCOL	U	U	Y	Y	L	L	Y	Y	U	U	F	--
9.	S.E. Ingle, et al.	REDEQL.EPA	U	U	Y	Y	N	U	Y	Y	U	U	F	--
10.	D.K. Harriss, et al.	REDEQL-UMD	U	U	Y	Y	N	L	Y	Y	U	U	F	--
11.	Y.K. Kharaka I. Barnes	SOLMNEQ	U	U	Y	Y	U	U	Y	Y	U	U	F	--
12.	B.W. Goodwin M. Munday	SOLMNQ	U	U	Y	Y	U	L	U	U	U	U	F	--
13.	J.W. Ball, et al.	WATEQ2	Y	U	Y	Y	N	Y	Y	Y	U	U	M	--
14.	J.W. Ball, et al.	WATEQ3	Y	U	Y	Y	U	L	Y	Y	U	U	M	--
15.	L.N. Plummer, et al.	WATEQF	Y	U	Y	Y	N	Y	Y	Y	U	U	M	3620

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	P.S. Huyakorn H.O. White T.D. Wadsworth Ref: 78	IGWMC Holcomb Research Institute 4600 Sunset Ave. Indianapolis, IN 46208	TRAFRAP-WT (1987)	A two-dimensional finite-element model to simulate transient, saturated groundwater flow and chemical or radionuclide transport in fractured or unfractured, anisotropic, heterogeneous, multilayered porous media; fractures handled by either the dual porosity or the discrete fracture approach.	Convection, dispersion, diffusion, adsorption, absorption, decay, reactions	0589
2.	P.S. Huyakorn Ref: 70	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	GREASE2 (1982)	A finite-element model to study transient, multidimensional, saturated groundwater flow, solute and/or energy transport in fractured and unfractured, anisotropic, heterogeneous, multilayered porous media.	Convection, conduction, dispersion, diffusion, adsorption	0582
3.	P.S. Huyakorn Ref: 81	Code Custodian Performance Assessment Dept. Office of Nuclear Waste Isolation Battelle Project Mgmt. Div. 505 King Avenue Columbus, OH 43201	STAFAN2 (1982)	A finite element model for simulation of transient two-dimensional flow and stress in deformable fractured and unfractured porous media.	Deformation	0584
4.	S.B. Pahwa B.S. Rama Rao Ref: 83	Code Custodian Performance Assessment Dept. Office of Nuclear Waste Isolation Battelle Project Management Div. 505 King Avenue Columbus, OH 43201	NETFLOW (1982)	A finite-element model to simulate steady-state three-dimensional flow in a heterogeneous medium by an equivalent network of series and parallel flow members		0695
5.	V. Guvanasen Ref: 24	Applied Geoscience Branch Whiteshell Nuclear Research Atomic Energy of Canada Pinawa, Manitoba Canada ROE 1LO	MOTIF (1986)	Finite-element model for one, two, and three-dimensional saturated/unsaturated groundwater flow, heat transport, and solute transport in fractured porous media, facilitates single-species radionuclide transport and solute diffusion from fracture to rock matrix.	Convection, dispersion, diffusion, adsorption, decay, advection	0953

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
6.	J.F. Pickens Ref: 56	INTERA Technologies, Inc. 6850 Austin Center Blvd., #300 Austin, TX 78731	FRACT (1981)	A finite-element model for simulation of advective-dispersive solute transport in linear fractures with solute diffusion into the adjacent matrix blocks.	Convection, dispersion, diffusion, adsorption, ion exchange, decay	2032
7.	J.F. Pickens Ref: 57	INTERA Technologies, Inc 6850 Austin Center Blvd., #300 Austin, TX 78731	FRACSOL (1981)	Analytical solution for simulation of solute transport in fractured media.	Convection, diffusion	2037
8.	K. Pruess Ref: 141	Mailstop 50E Lawrence Berkeley Lab Berkeley, CA 94720	MULKOM (1985)	Multicomponent, multiphase fluid and heat flow in porous or fractured media; MINC concept, separate equations for flow through matrix and fractures. Fractures are represented by one-dimensional cells.	Convection, change of phase, dissolution and precipitation of silica, equilibration of noncondensible gases, transport of noncondensible gases and dissolved solids.	2581
9.	K. Pruess Y.W. Tsang J.S.Y. Wang	Earth Sciences Division Lawrence Berkeley Laboratory University of California Berkeley, CA 94720	TOUGH (1984)	An integrated-finite-difference model for transient simulation of two-phase flow of water and air with simultaneous heat transport in fractured unsaturated porous media.	Condensation, capillary forces, evapotranspiration, conduction, diffusion, change of phase, adsorption, compression, dissolution of air in liquid, advection, buoyancy	2582
10.	J. Noorishad P.A. Witherspoon	Earth Sciences Division Lawrence Berkeley Laboratory Univ. of California Berkeley, CA 94720	ROCMAS-H (1976)	A finite-element model for two-dimensional simulation of transient ground water flow in porous fractured rock.		3080
11.	J. Noorishad M. Menran Ref: 123	Earth Sciences Division Lawrence Berkeley Laboratory Univ. of California Berkeley, CA 94720	ROCMAS-HS (1981)	A transient model to solve for two-dimensional dispersive-convective transport of nonconservative solutes in saturated, fractured porous media for a given velocity field as generated by ROCMAS-H.	Convection, dispersion, diffusion, adsorption, decay, reactions	3081

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
12.	J. Noorishad M.S. Ayatollahi P.A. Witherspoon Ref: 124	Earth Sciences Division Lawrence Berkeley Laboratory Univ. of California Berkeley, CA 94720	ROCMAS-HM (1981)	Two-dimensional finite-element model for analysis of quasi-static coupled stress and fluid flow in porous fractured rock.	Consolidation, fracture deformation	3082
13.	J. Noorishad P.A. Witherspoon Ref: 193	Earth Science Div. Lawrence Berkeley Lab. Univ. of California Berkeley, CA 94720	ROCMAS-THM	Two-dimensional finite-element model for coupled hydraulic-thermal-mechanical analysis of porous fractured rock.	Convection, conduction, consolidation	3083
14.	B. Sagar Ref: 52	Analytic & Computational Research, Inc. 3106 Inglewood Blvd. Los Angeles, CA 90066	FRACFLOW (1981)	Integrated-finite-difference model for steady and unsteady state analysis of density-dependent flow, heat and mass transport in fractured confined aquifers; two-dimensional simulation of the processes in the porous medium and one-dimensional simulation of the fractures.	Convection, conduction, dispersion, diffusion, consolidation adsorption, decay, reactions	3232
15.	D.L. Deangelis G.T. Yeh D.D. Huff Ref: 34	Environmental Sciences Division Oak Ridge National Laboratory Oak Ridge, TN 37830	FRACPORT (1984)	An integrated compartmental model for describing the transport of solute in a fractured porous medium.	Dispersion, adsorption, decay, advection	3374
16.	O.D.L. Strack Ref: 161	R.W. Nelson Battelle Pacific Northwest Laboratories Hydrologic Systems Section Richland, WA 99352	BACRACK (1982)	A boundary element model to simulate two-dimensional steady flow through fissured porous media.		3440
17.	N.W. Kline R.L. England R.C. Boca Ref: 94	Rockwell International Rockwell Hanford Operations P.O. Box 800 Richland, WA 99352	CHAINT (1985)	A general purpose two-dimensional, finite-element model for radionuclide transport in a fractured porous medium. Requires output of the finite-element flow model MAGNUM 2D as input.	Dispersion, diffusion, adsorption, decay, advection, buoyancy, chain-decay (two daughters)	3791
18.	A.L. Edwards A. Rasmuson I. Neretnieks T.N. Narasimhan Ref: 38	Dept. of Chemical Engineering Royal Inst. of Technology S-100 44 Stockholm, Sweden	TRUMP (1980)	A multidimensional model based on the integrated-finite-difference method, to simulate steady-state or transient ground water flow and heat or solute transport in fractured rock.	Conduction, dispersion, diffusion, decay, advection	4030

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
19.	A. Rasmuson I. Neretnieks Ref: 115	Dept. of Chemical Engineering Royal Institute of Technology S-100 44 Stockholm, Sweden	TRUCHN/ZONE (1984)	Advection-dispersion of radionuclides in strongly fissured zones including diffusion into the rock matrix with strongly varying velocity and block sizes along the flow path.	advection, dispersion, diffusion into rock	4031
20.	B.J. Travis Ref: 170	Earth and Space Sciences Division Los Alamos National Laboratory Los Alamos, NM 87545	TRACR3D (1984)	A three-dimensional finite-difference model of transient two-phase flow and multicomponent transport in deformable, heterogeneous, reactive porous/fractured media.	Dispersion, diffusion, adsorption, decay, advection	4270
21.	K. Karasaki Ref: 87	Earth Sciences Division Lawrence Berkeley Lab. University of California Berkeley, CA 94720	FRACTEST (1986)	Simulation of flow in fractured rock for well test analysis. The model consists of a mesh generator to produce a representative fractured system and a finite-element model for calculation of transient hydraulic heads using a parallel processor.		4470
22.	S.A. Holditch and Associates Ref: 69	U.S. Department of Energy Office of Fossil Energy Morgantown Energy Technolgy Center P.O. Box 880 Morgantown, WV 26505	SUGARWAT (1983)	A two-dimensional, two-phase finite-difference model to simulate the transient flow of both gas and water in dual porosity reservoirs.	Gas desorption from pore wells	4490
23.	L. Kiraly Ref: 92	National Cooperative for Storage of Radioactive Waste-NAGRA Parkstrasse 23 CH-5401 Baden Switzerland	FEM3D1 (1985)	A three-dimensional finite-element model for simulation of steady-state flow in an equivalent anisotropic porous medium intersected by linear or planar discontinuities.		4500
24.	V. Guvanasen Ref: 66	Tin Chan AECL Whiteshell Nuclear Research Establishment Pinawa, Maintoba Canada	MOTIF (1987)	A finite-element model to simulate the coupled processes of saturated or unsaturated fluid flow, conductive and convective heat transport, brine transport and single species radionuclide transport in a compressible rock of low permeability intersected with fractures.	Capillary forces, convection, conduction, dispersion, diffusion, consolidation, hysteresis, adsorption, ion exchange, decay, reactions	4550

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
25.	J.D. Miller	Hydrology Unit Idaho National Engineering Lab Idaho Falls, ID 83415	FRACSL (1986)	A steady-state two-dimensional finite-difference model to simulate flow and solute and heat transport in a porous rock with discrete fractures.	advection, diffusion, dispersion, conduction	4670
26.	P.S. Huyakorn Ref: 71	HydroGeoLogic, Inc. 503 Carlisle Dr., Suite 250 Herndon, VA 22070	STAFF2D (1988)	A two-dimensional finite-element model to simulate flow and solute transport in fractured or granular porous media. The model can address both confined and unconfined formations, and it can handle fracture systems containing an intricate network of fractures and/or a few discrete fractures.	infiltration, aquitard leakage, advection, dispersion, adsorption, degradation	4710
27.	E.A. Sudicky Ref: 162	Institute for Groundwater Research Dept. of Earth Sciences University of Waterloo Waterloo, Ontario Canada N21 3G1	CRACK (1986)	A package of four analytical models for mass transport in fractured porous media. The models address transport in a single fracture with matrix diffusion and transport in a network of parallel fractures.	dispersion along fracture axis; matrix diffusion	6660

APPENDIX F2 FRACTURED ROCK MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
1.	P.S. Huyakorn, et al.	TRAFRAP-WT	N	N	Y	Y	N	Y	Y	Y	Y	L	F	0589
2.	P.S. Huyakorn	GREASE2	N	N	Y	Y	L	L	Y	Y	Y	L	F	0582
3.	P.S. Huyakorn	STAFAN2	N	N	Y	Y	L	L	Y	Y	Y	U	F	0584
4.	S.B. Pahwa B.S. Rama Rao	NETFLOW	U	U	Y	Y	L	L	U	U	Y	U	F	0695
5.	V. Guvanasen	MOTIF	U	U	Y	Y	N	L	U	U	Y	L	F	0953
6.	J.F. Pickens	FRACT	N	N	N	N	L	N	U	U	Y	U	F	2032
7.	J.F. Pickens	FRACSOL	N	N	N	N	L	N	U	U	Y	U	F	2037
8.	K. Pruess	MULKOM	N	N	N	N	L	N	U	U	Y	U	F	2581
9.	K. Pruess, et al.	TOUGH	N	N	N	N	U	N	U	U	Y	U	F	2582
10.	J. Noorishad P.A. Witherspoon	ROCMAS-H	U	U	Y	Y	U	L	Y	Y	Y	U	F	3080
11.	J. Noorishad M. Menran	ROCMAS-HS	U	U	Y	Y	U	L	Y	Y	Y	U	F	3081
12.	J. Noorishad M.S. Ayatollahi P.A. Witherspoon	ROCMAS-HM	U	U	Y	Y	U	L	Y	Y	Y	U	F	3082
13.	J. Noorishad P.A. Witherspoon	ROCMAS-THM	U	U	Y	Y	U	L	Y	Y	Y	U	F	3083
14.	B. Sagar	FRACFLOW	N	N	Y	Y	N	L	U	U	Y	U	F	3232
15.	D.L. Deangelis, et al.	FRACPORT	N	N	Y	Y	L	L	U	U	Y	U	F	3374
16.	O.D.L. Strack	BACRACK	N	N	N	N	Y	L	Y	Y	Y	L	F	3440
17.	N.W. Kline, et al.	CHAINT	U	U	Y	Y	Y	L	U	U	Y	L	F	3791
18.	A.L. Edwards	TRUMP	U	U	Y	Y	U	N	U	U	Y	U	F	4030

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

APPENDIX F2 FRACTURED ROCK MODELS: USABILITY AND RELIABILITY

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
19.	A. Rasmuson I. Neretnicks	TRUCHN/ ZONE	U	U	Y	Y	U	L	U	U	Y	U	F	4031
20.	B.J. Travis	TRACR3D	U	U	Y	Y	L	L	Y	Y	Y	L	F	4270
21.	K. Karasaki	FRACTEST	N	N	N	N	Y	N	U	U	Y	L	F	4470
22.	S.A. Holditch & Associates	SUGARWAT	U	U	Y	Y	U	U	U	U	Y	L	F	4490
23.	L. Kiraly	FEM301	U	U	N	N	U	U	U	U	Y	L	F	4500
24.	V. Guvanasen	MOTIF	U	U	N	N	U	U	U	U	Y	L	F	4550
25.	J.D. Miller	FRACSL	U	U	Y	Y	U	L	Y	U	Y	U	F	4670
26.	P.S. Huyakorn	STAFF2D	N	N	Y	Y	N	Y	Y	U	Y	L	F	4710
27.	E.A. Sudicky	CRACK	D	Y	Y	Y	L	L	Y	U	Y	L	F	6660

KEY: Y = YES N = NO U = UNKNOWN G = GENERIC D = DEDICATED L = LIMITED M = MANY F = FEW

APPENDIX G1 MULTIPHASE FLOW MODELS: SUMMARY LISTING

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
1.	C.R. Faust J.W. Mercer Ref: 48	Performance Assessment Dept Office of Nuclear Waste Isolation Battelle Project Mgmnt. Div. 505 King Avenue Columbus, OH 43201	GEOTHER (1983)	A finite-difference model for simulation of transient, three-dimensional, single and two-phase heat transport in anisotropic, heterogeneous, permeable media.	Condensation, convection, conduction, dispersion, diffusion, change of phase	0730
2.	J.H. Guswa D.R. LeBlanc Ref: 64	U.S. Geological Survey 150 Causeway St. Suite 1001 Boston, MA 02114	Cape Cod Aquifer System Models (1981)	Steady-state simulation of three-dimensional flow in a heterogeneous, anisotropic aquifer with a sharp static interface between fresh and salt water.	interface	0770 mod.
3.	M. Clouet D'Orval	Burgeap 70, Rue Mademoiselle 75015 Paris France	BURGEAP 7600HYSO PACKAGE (1982)	A program package to simulate two-dimensional, horizontal/vertical, steady/transient, saturated flow in confined/unconfined, homogeneous/heterogeneous aquifer systems with multiple imiscible fluids, and connection with surface water.		1370
4.	M. Clouet D'Orval	Burgeap 70, Rue Mademoiselle 75015 Paris France	BURGEAP 7600HYSO (TRABISHA MODEL) (1981)	To simulate two-dimensional, horizontal, transient, saturated flow of two immiscible fluids of different densities, in unconfined, homogeneous/heterogeneous aquifers.		1371
5.	W. Giesel G. Schmidt K. Trippler Ref: 156	Bundesanstalt für Geowissenschaften und Rohstoffe P.O. Box 510153 3000 Hannover 51 West Germany	Aquifer Simulation Subroutines Package (1976)	Finite-difference simulation of steady-state or transient groundwater flow in an anisotropic, heterogeneous, multi-aquifer system, including a saltwater/freshwater interface.		1550
6.	P. van der Veer Ref: 181	Rijkswaterstaat, Data Processing Division P.O. Box 5809 2280 HB Rijswijk (Z.H.) The Netherlands	MOTGRO (1981)	Prediction of groundwater head and stream function for two-dimensional, vertical, steady and unsteady single or multiple fluid flow in inhomogeneous, anisotropic, confined or unconfined aquifers of arbitrary shapes; uses analytical function method.		1830

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
7.	A. Verruijt J.B.S. Gan Ref: 186	Techn. Univ. Delft Dept. Civil Engineering Stevinweg 1 2628 CN Delft The Netherlands	SWIFT (1982)	A cross-sectional finite-element model for transient, horizontal flow of salt and fresh water and analysis of upconing of an interface in a homogeneous aquifer.	upconing	1852
8.	J.W. Mercer C.R. Faust Ref: 109	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	SWSOR (1980)	A two-dimensional finite-difference solution to simulate the areal, unsteady flow of saltwater and freshwater separated by an interface in anisotropic, heterogeneous porous media.		2140
9.	K. Pruess Ref: 141	Mailstop 50E Lawrence Berkeley Lab Berkeley, CA 94720	MULKOM (1985)	Multicomponent, multiphase fluid and heat flow in porous or fractured media.	Convection, change of phase, dissolution and precipitation of silica, equilibration of noncondensible gases, transport of noncondensible gases and dissolved solids.	2581
10.	K., Y.W. Pruess J.S.Y. Wang	Earth Sciences Division Lawrence Berkeley Laboratory University of California Berkeley, CA 94720	TOUGH (1984)	An integrated-finite-difference model for transient simulation of two-phase flow of water and air with simultaneous heat transport in fractured unsaturated porous media.	Condensation, capillary forces, evapotranspiration, conduction, diffusion, change of phase, adsorption, compression, dissolution of air in liquid, advection, buoyancy	2582
11.	A.A.G. Sada Costa J.L. Wilson	Director, R.M. Parsons Laboratory for Water Resources and Hydrodynamics Dept. of Civil Engineering MIT Cambridge, MA 02139	SWIM (1981)	A versatile finite-element model to simulate transient, horizontal salt and fresh water flow in porous media, separated by a sharp interface.		2631

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
12.	R.H. Page Ref: 126	Water Resources Program Dept. of Civil Engineering Princeton University Princeton, NJ 08540	INTERFACE (1979)	A finite-element model to simulate transient flow of fresh and saline water as immiscible fluids separated by an interface in an isotropic, heterogeneous, water-table aquifer.		2720
13.	J.W. Pritchett Ref: 139	Systems, Science and Software P.O. Box 1620 La Jolla, CA 92038	MUSHRM (1980)	A finite-difference multi-species hydrothermal reservoir model to simulate unsteady multiphase fluid and heat flow in mutidimensional geometries.	Convection, conduction, change of phase, degassing phenomena	2760
14.	J.W. Pritchett	Systems, Science and Software P.O. Box 1620 La Jolla, CA 92038	CHARGR (1980)	Multispecies hydrothermal reservoir model to simulate unsteady multiphase fluid and heat flow in multidimensional geometries by means of finite-difference method.	Heat convection and conduction; degassing; consolidation; expansion; change of phase (flow is coupled)	2761
15.	D.N. Contractor Ref: 194	Water and Energy Research Inst. of The Western Pacific University of Guam College Station, Mangilao, Guam 96913	SWIGS2D (1982)	A two-dimensional finite-element model to simulate transient, horizontal salt and fresh water flow separated by a sharp interface in an anisotropic, heterogeneous, confined, semi-confined or water-table aquifer.		3600
16.	R.I. Allayla Ref: 3	Civil Eng. Dept. Colorado State Univ. Fort Collins, CO 80523	SEAWTR/ SEACONF (1980)	A two-dimensional finite-difference model for horizontal simulation of simultaneous flow of salt and fresh water in a confined or water-table aquifer with anisotropic and heterogeneous properties, including effects of capillary flow.	Capillary forces, influence of capillary region on specific yeild	3640
17.	A.L. Baehr Ref: 7	U.S.G.S. Water Resources Div. National Center 12201 Sunrise Valley Dr. Reston, VA 22092	GASOLINE (1984)	A one-dimensional model to solve a system of equations defining the transport of an immiscible contaminant immobilized in the unsaturated zone, with or without biodegradation.	Capillary forces, dispersion, diffusion, adsorption, reactions, advection, buoyancy, biological activity	4420

No.	Author(s)	Contact Address	Model Name (last update)	Model Description	Model Processes	IGWMC Key
18.	S.A. Holditch And Associates Ref: 69	Office of Fossil Energy, Morgantown Energy Technology Center, P.O.880, Morgantown, WV 26505	SUGARWAT (1983)	A two-dimensional, two-phase finite-difference model to simulate the transient flow of both gas and water in dual porosity reservoirs.	Gas desorption from pore wells	4490
19.	C.R. Faust J.D. Rumbaugh Ref: 49	GeoTrans, Inc. 250 Exchange Place Suite A Herndon, VA 22070	SWANFLOW (1986)	Three-dimensional simulation of flow of water and immiscible non-aqueous phase liquids within and below the vadose zone with a finite difference solution.	Capillary forces	4650

No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
1.	C.R. Faust J.W. Mercer	GEOTHER	N	N	Y	Y	L	L	U	U	Y	L	F	0730
2.	J.H. Guswa D.R. LeBlanc	Cape Cod Aquifer Systems Model	N	N	Y	Y	N	U	U	U	Y	U	F	0770 mod.
3.	M. Clouet D'Orval	BURGEAP 7600 HYSO PACKAGE	N	N	Y	Y	Y	N	U	U	Y	Y	M	1370
4.	M. Clouet D'Orval	TRABISA	N	N	Y	Y	Y	N	U	U	U	Y	M	1371
5.	W. Giesel, et al.	Aquifer Simulation Subroutines Package	N	N	N	N	U	N	U	U	U	L	F	1550
6.	P. van der Veer	MOTGRO	N	N	Y	Y	L	U	U	U	Y	L	F	1830
7.	A. Verruijt J.B.S. Gan	SWIFT	N	N	Y	Y	N	L	Y	U	Y	U	F	1852
8.	J.W. Mercer C.R. Faust	SWSOR	N	N	Y	Y	N	L	Y	Y	Y	L	F	2140
9.	K. Pruess	MULKOM	N	N	N	N	L	N	U	U	Y	U	F	2581
10.	K. Pruess, et al.	TOUGH	N	N	N	N	U	N	U	U	Y	U	F	2582
11.	A.A.G. Sada Costa	SWIM	N	N	U	U	U	U	U	U	Y	L	F	2631
12.	R.H. Page	INTERFACE	N	N	Y	Y	L	N	U	U	Y	L	F	2720
13.	J.W. Pritchett	MUSHRM	U	U	Y	Y	U	U	U	U	Y	L	U	2760
14.	J.W. Pritchett	CHARGR	U	U	Y	Y	N	Y	Y	U	Y	U	F	2761
15.	D.N. Contractor	SWIGS2D	U	U	Y	Y	U	L	U	U	Y	L	F	3600
16.	R.I. Allayla	SEAWTR/ SEACONF	N	N	Y	Y	L	N	U	U	Y	L	F	3640

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No.	Author(s)	Model Name	USABILITY						RELIABILITY					IGWMC KEY
			Preprocessor	Postprocessor	User's Instructions	Sample Problems	Hardware Dependency	Support	Peer Reviewed Theory	Peer Reviewed Coding	Verified	Field Tested	Model Users	
17.	A.L. Baehr	GASOLINE	N	N	Y	Y	U	L	Y	Y	Y	L	F	4420
18.	S.A. Holditch & Associates	SUGARWAT	U	U	Y	Y	U	U	U	U	Y	L	F	4490
19.	C.R. Faust J.D. Rumbaugh	SWANFLOW	Y	Y	Y	Y	L	L	U	U	Y	L	F	4650

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