CONCEPTUAL AND MATHEMATICAL MODELING
OF THE HANFORD GROUNDWATER FLOW REGIME

R. C. Arnett
R. A. Deju
R. W. Nelson[†]
C. R. Cole^{*}
R. E. Gephart

Research Department
Research and Engineering Division

[†]Scientific Systems Department
Boeing Computer Services Richland, Inc.
Richland, Washington

^{*}Water and Land Resources Department
Battelle, Pacific Northwest Laboratories
Richland, Washington

October 1976

ATLANTIC RICHFIELD HANFORD COMPANY
RICHLAND, WASHINGTON 99352

MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ABSTRACT

Disposal of radioactive wastes to surface disposal sites at the Hanford Atomic Reservation has resulted in some radioactive and chemical contamination of the underlying groundwater flow systems. In support of the Hanford groundwater management effort a preliminary conceptual model of the groundwater system has been formulated as a first step in understanding possible contaminant movement. The mathematical modeling capabilities needed for better understanding and prediction of such contaminant movement are discussed in this paper and the state-of-the-art in groundwater modeling as related to Hanford is summarized with emphasis upon computer solution methods. An inventory of potentially applicable codes available both at Hanford and elsewhere is included. The areas where groundwater modeling capability is lacking are outlined and the steps needed to overcome such deficiencies discussed.

TABLE OF CONTENTS

ABSTRACT	iii
FIGURES	v
TABLES	vi
INTRODUCTION	1
PURPOSE	1
MODELING	2
CONCEPTUAL MODEL	5
FROM THE CONCEPTUAL MODEL TO THE MATHEMATICAL MODELS	13
MATHEMATICAL MODELS	19
GENERAL MODEL ASSUMPTIONS	20
FLOW OF IMMISCIBLE FLUIDS (MULTIPHASE FLOW)	23
PARTIALLY SATURATED FLOW	37
SATURATED, CONFINED FLOW	40
SATURATED, UNCONFINED OR FREE SURFACE FLOW MODEL	42
BOUSSINESQ TYPE FLOW	46
CONTAMINANT TRANSPORT	53
MATHEMATICAL SOLUTION METHODS FOR FLOW AND TRANSPORT PROBLEMS	61
SELECTED COMPUTER CODES POTENTIALLY APPLICABLE TO HANFORD	62
FLUID FLOW DETERMINATIONS	63
CONTAMINANT TRANSPORT ANALYSIS	67
NUMERICAL METHODS OF OBTAINING IMPROVED DATA DISTRIBUTIONS	67
AUXILIARY COMPUTER CODES	69
CONCLUSIONS AND RECOMMENDATIONS	71
REFERENCES	73
APPENDIX - MODEL INVENTORY	75
APPENDIX REFERENCES	98
ACKNOWLEDGMENTS	103

FIGURES

FIGURE 1	MODEL UTILIZATION AT THE HANFORD RESERVATION	4
FIGURE 2	MAP OF THE PASCO BASIN INCLUDING THE HANFORD RESERVATION	6
FIGURE 3	CROSS-SECTION MAP OF THE HANFORD RESERVATION SHOWING THE NATURAL AND WASTE DISCHARGE FLOW SYSTEMS	10
FIGURE 4	SIMPLIFIED CONCEPTUAL MODEL OF THE HANFORD RESERVATION	12
FIGURE 5	MODELING FRAMEWORK.	16
FIGURE 6	DATA REQUIREMENTS	17
FIGURE 7	FLUID FLOW EQUATION FORMULATIONS TO BE DISCUSSED . .	21
FIGURE 8	TYPE OF TRANSPORT EQUATION FORMULATIONS TO BE DISCUSSED	22
FIGURE 9	DIAGRAM OF A POROUS MEDIUM WITH TWO IMMISCIBLE FLUIDS .	24
FIGURE 10	IDEALIZED GRAPH OF CAPILLARY PRESSURE, P_c , VERSUS S_1 AND S_2 SHOWING THE HYSTERESIS PHENOMENA	26
FIGURE 11	TYPICAL RELATIVE PERMEABILITIES OF GAS (1) AND WATER (2) FOR UNCONSOLIDATED SAND AS A FUNCTION OF SATURATION .	30
FIGURE 12	OFFSITE AND ONSITE FLOW MODELS OF POTENTIAL USE AT HANFORD	64
FIGURE 13	OFFSITE AND ONSITE TRANSPORT MODELS OF POTENTIAL USE AT HANFORD	68

TABLES

TABLE 1	GENERAL DATA REQUIREMENTS	18
---------	-------------------------------------	----

CONCEPTUAL AND MATHEMATICAL MODELING OF THE HANFORD GROUNDWATER FLOW REGIME

INTRODUCTION

PURPOSE

Since 1944 the Hanford Reservation, located in south-central Washington, has been a site for radioactive waste storage, reactor development, and chemical separation facilities for the production and purification of plutonium needed in the development of nuclear weapons.^[1] These activities have involved the disposal of some radioactive waste to surface or near surface disposal sites with a consequent contamination of some of the aquifers underlying the Hanford Reservation. An extensive groundwater monitoring program conducted over the years at Hanford indicates that the movement of radioactive contaminants through the groundwater flow system toward biosphere uptake points (primarily the Columbia River) is limited. Nevertheless, a program is being conducted to assure continued isolation of such contaminants from the biosphere both now and in the future.

At present, the Atlantic Richfield Hanford Company operates the waste management activities at Hanford under contract to the U.S. Energy Research and Development Administration. A Groundwater Management program has been instituted in support of the waste management activities to: (1) identify potential ways in which groundwater can come in contact with high-level radioactive wastes; (2) identify existing computer codes and models useful in predicting consequences of accidental and planned radioactive waste releases to the groundwater; (3) assess data-gathering requirements needed for long-term prediction of subsurface contaminant migration from high-level radioactive waste areas into and through the groundwater flow system; and (4) examine potential impact to the high-level waste areas resulting from past, present, and projected activities at Hanford, potentially hazardous incidents, and potential or existing water usage adjacent to or within the Hanford Reservation. The purpose of this report is to (1) discuss the modeling capabilities needed in support of the above-mentioned groundwater management objectives, (2) summarize the state-of-the-art in modeling, and (3) design a program that incorporates all needed modeling technology to satisfy the needs at the Hanford Reservation.

MODELING

A model can be defined as a simplified representation of a given system. Models must behave in a manner analogous to the actual system under a set of specified conditions. The objective of constructing a model is usually to assess the impact of certain actions and/or conditions on the actual system.

In general terms, models can be classed into four groups: conceptual, scaled, analog, and mathematical. A conceptual model is nothing more than a word-description of the actual system. Such models form the basis for a preliminary understanding of the actual system and can be used in defining more sophisticated models of the system. Scaled models are physical facsimiles of the full-scale prototype.^[2] Analog models describe a system's behavior by describing the response of an analogous system to a given set of input variables.^[3]

Mathematical models are representations of a system by means of a set of equations satisfying a number of conditions which occur in the actual system. Mathematical models can be further classed into two groups: stochastic and deterministic. Stochastic models are such that one or more variable in the system is regarded as random or as Kisiel^[4] defines them: "In the stochastic approach uncertainty by way of probability laws is woven onto the fabric of hydrodynamic and phenomenological relations which define mean-value behaviour of a system with zero mean-square error." Deterministic models, on the other hand involve only variables that are free from random variation.

Mathematical models are useful in our Hanford groundwater management effort. Such models can provide the waste manager a tool which can be used to assess the effects of waste strategies on the Hanford groundwater regime. They can also be used to define corrective actions which might be taken as a result of an accidental release of contaminants into the groundwater regime. Overall, the purpose of the models is not only to further characterize the flow system but also to teach us how to

manage the groundwater regime and methods of controlling an accidental release of radioactive waste and preventing its reaching the biosphere. Models developed at Hanford are used in an environmental assessment of a hydrologic problem or as required to make a waste management decision (Figure 1).

In order to utilize mathematical modeling effectively at Hanford for groundwater management purposes, one must:

- understand the physical and chemical processes which occur while the waste is moving from the discharge point through the soil and the groundwater system or systems to the surface water discharge sites or other biosphere uptake points;
- identify and determine the physical and chemical parameters which allow one to solve the equations governing the physical and chemical processes which occur throughout the waste path;
- characterize all past, current, and future waste sources and identify and characterize their associated groundwater entry mechanisms;
- characterize the current condition of the groundwater regime; and
- identify system boundary conditions, including all points of biosphere uptake.

While different models will require different amounts and types of data, any mathematical model is only as good as our conceptual understanding of the actual system. One needs to begin by developing a basic conceptual model of the actual system and then assessing what mathematical models are best suited to describing each portion of the actual system.

V7606-23.1

FIGURE 1
MODEL UTILIZATION AT THE HANFORD RESERVATION

CONCEPTUAL MODEL

The Hanford Reservation is located in the Columbia Plateau basaltic province of south-central Washington. The Reservation covers 576 square miles (1492 km²) within the structural and topographic low called the Pasco Basin. The Basin was formed by the slow subsidence of the underlying crust resulting from the withdrawal of large volumes of lava which flowed back into the Basin. Today, the Pasco Basin is bordered on the north by the Saddle Mountains, Umtanum and Yakima Ridges on the west, the Rattlesnake Hills and the Horse Heaven Hills on the south and on the east by a broad monoclinal arch (Figure 2).

A series of basaltic flows known as the Columbia River Basalts were extruded into the Pasco Basin during the Miocene and Pliocene geologic epochs. Fluvial and lacustrine sediments were deposited between lava outpourings. These sedimentary rocks form an extensive regional flow system through which ground water flows.

Concurrent with the lava outpourings, north-south compressional forces folded the basalts into a sequence of east-west trending anticlinal and synclinal folds. The principal anticlinal structure crossing the Hanford Reservation is the Umtanum-Gable Anticline. Flanking this anticline are the Cold Creek and Pasco Synclines, which form two sub-basins in the larger Pasco Basin (Figure 2). Several hundred feet of Pliocene and Pleistocene sediments now fill these synclines.

The sedimentary rocks overlying the Columbia River Basalts consist of the Ringold Formation and glaciofluvial material. The Ringold is made of intergrading and interlensing sequences of sands, silts, and gravels. It is frequently described as consisting of an upper silty sand, middle conglomerates, and a lower clay horizon. The lower clay horizon commonly contains sand and gravel lenses. However, this three unit division is a simplification of rather complex stratigraphic

FIGURE 2
MAP OF THE PASCO BASIN INCLUDING THE HANFORD RESERVATION

relationships in which individual geologic units may be difficult to correlate due to frequent facies changes. Some formational boundaries are sharp but most are gradational.

The Pleistocene deposits consist of eolian silts and glaciofluvial sediments. The eolian silts mark the boundary between the Ringold Formation and the overlying deposits. The glaciofluvial deposits consist of coarse-grained sands, pebbles and cobbles. These were deposited in glacial meltwaters flooding the Pasco Basin during the last ice age. Throughout most of the Hanford Reservation, these Pleistocene deposits lie atop a thick sequence of Ringold sediments. However, in some areas such as along the Umtanum-Gable Anticline, the Ringold has been deeply eroded or completely removed. Between Gable Butte and Gable Mountain, glaciofluvial sediments overlie a highly deformed and deeply eroded sequence of Columbia River Basalts.

The most permeable horizons in the Ringold Formation are the sands and conglomerates of the upper and middle Ringold units. Fractures and intergranular porosity may both be significant factors in controlling groundwater flow through these units. Individual clay lenses and cemented zones within the Ringold may act as local aquitards but appear to have negligible impact on the overall groundwater flow regime. The glaciofluvial sediment possesses the highest permeability of all sediment beneath the Hanford Reservation.

The shallowest aquifer beneath the Hanford Reservation lies within the glaciofluvial sediment and the Ringold Formation. Its upper boundary is defined by the regional water table and its lower boundary by the lower Ringold clays or the Columbia River basalt. Beneath most of the areas where high-level wastes are stored (200 W and 200 E Areas, Figure 2), the water table lies within the Ringold Formation. Toward the Columbia River, the water table rises above the Ringold and intersects the overlying glaciofluvial sediment. The general groundwater flow is to the east and southeast where it discharges into the Columbia River.

In the area from Umtanum Ridge to the Rattlesnake Hills, ground water from the regional flow system recharges the overlying sediments that form the unconfined aquifer underlying the Hanford Reservation. In addition, the unconfined aquifer has been contaminated with liquid wastes disposed at several ponds within the Hanford Reservation. The total volume of liquid wastes disposed since operations began exceeds 150 billion gallons (600 billion liters) the overwhelming bulk of which is low level waste (less than 5×10^{-5} microcuries per milliliter). In the last ten years disposal volumes have ranged from 5.3 to 8 billion gallons/year (20 to 30 billion liters/year). The bulk of the liquid waste is discharged to five sites (Figure 2): (1) Gable Mountain pond (216-A-25), (2) 216-B-3 pond, (3) 216-S-19 pond, (4) 216-T-4 pond, and (5) 216-U-10 pond. In the 300 Area (laboratory facilities just north of Richland) the liquid waste disposal rate averages 1 billion gallons/year (4 billion liters/year).

Pond disposal contributes the bulk of the waste recharge into the unconfined groundwater flow system underlying the Hanford Reservation. Water disposed at the ponds contains low levels of radioactivity. In addition, waste disposal through cribs and specific retention sites contributes both water and contamination to the groundwater flow system. The total volume of liquid received by a crib may be as little as a few thousand liters in the cribs used for a short period of time or as much as 260 million gallons (1 billion liters) in those cribs which have seen sustained service for many years. Although the cribs and specific retention sites contribute only small volumes of water to the groundwater flow regime they do contribute a significant portion of the radionuclide inventory introduced into the groundwater pathway.

Flow beneath the Hanford water table occurs under conditions of full saturation. The direction and rate of flow between any two points in this continuum is controlled by the potential (head) difference between the two points and the hydraulic properties of the porous medium and fluid.

The Hanford hydrologic regime is basically a combination of two natural flow systems and a waste discharge system. Figure 3 depicts

these systems along a cross section through the Reservation. This figure is based upon piezometric data.

The uppermost local flow systems resulting from the waste disposal operations appear to overlie and interact with the natural intermediate system composed of Ringold and glaciofluvial sediment. The lower boundaries of the local systems are groundwater divides extending from the waste recharge areas to the discharge points. The local flow systems increase in size as the rate of waste disposal increases and shrink as the disposal activities are reduced. As shown in Figure 3, the local regime is composed of two subsystems associated with the 200 East and 200 West area discharges. The average hydraulic gradient beneath the 200 West Area is approximately 30 feet/mile and that beneath the 200 East Area is 15 feet/mile.

Ground water flows within the Ringold-glaciofluvial sediment as part of an intermediate system atop the regional flow continuum of the basalt aquifers. Prior to Hanford waste disposal, this system extended from the water table downward to the Ringold clays or the top of the Columbia River Basalts. At this time, the hydraulic gradient in all but the southwesternmost portion of the Hanford Reservation was approximately 5 feet/mile. Water discharges since 1944 at Hanford have raised the water table and altered the existing hydraulic gradients. Today, ground water flows radially outward from groundwater mounds formed beneath both 200 Areas.

Underlying the intermediate system is a regional flow system consisting of individual basaltic interbeds. The uppermost interbeds appear to recharge along ridges and plateaus fringing the Pasco Basin and discharge into the Columbia River adjacent to or south of the Hanford Reservation. Although detailed piezometric data are lacking, ground water movement in this regional system appears to be to the east and southeast beneath the Reservation. The regional system is in

FIGURE 3
CROSS-SECTION MAP OF THE HANFORD RESERVATION SHOWING
THE NATURAL AND WASTE DISCHARGE FLOW SYSTEMS

apparent isostatic equilibrium with the intermediate regime and the Columbia River along the eastern portion of the Hanford Reservation. This would be expected along a discharge area. In regions of breaching or severe tilting of the basalt flows as between Gable Butte and Gable Mountain, the regional flow system is in equilibrium with the overlying intermediate system, and possibly the local waste discharge system as well. Areas of sharp monoclinial down folding as in Cold Creek Valley act as flow barriers and increase the confining pressures in the regional system.

The point of introduction of radioactive or chemical wastes into the Hanford subsurface is almost always near the land surface. This is true whether the liquid waste discharge is a planned disposal such as to a pond or an accidental release. The distance from the near-surface discharge zone to the saturated flow system varies from several hundred feet to less than 50 feet. In any case, the initial portion of the waste path is likely to be within the partially saturated zone where a vapor-air phase coexists with and influences the movement of the liquid water phase. Under a sufficient driving force, some portion of the liquid will flow downward until it reaches the saturated zone where the influence of the vapor-air phase is restricted to the interface between the saturated and unsaturated zones (Figure 4). The waste liquid flow path within the saturated zone follows the local flow system described earlier. The waste liquid can come into contact with the intermediate flow regime along the groundwater divide separating the local waste discharge and intermediate flow systems. Introduction of waste liquid into the lower regional flow system can only occur where the basalt aquifers are in contact with the local waste discharge flow system and where pressure differences allow flow to move into the lower aquifers.

In addition to the physical description of the flow path, several physicochemical processes must be understood in order to assess waste transport. At Hanford the most important processes are chemical

V7606-23.2

FIGURE 4
SIMPLIFIED CONCEPTUAL MODEL OF THE HANFORD RESERVATION

reactions, dispersion, and radioactive decay. These processes vary depending on both the waste type and the sediment through which the waste flows. Temperature differences do not appear to play a significant role except in treating an accidental release from a waste tank or pipeline rupture where a highly nonisothermal situation prevails.

FROM THE CONCEPTUAL MODEL TO THE MATHEMATICAL MODELS

To understand the conceptual model that we have outlined and to satisfy our previously discussed management objectives we need to develop some mathematical models that represent the conceptual model or a portion of it.

Associated with each level of sophistication in a mathematical model is a data level requirement to adequately characterize the system. Generally as the mathematical model becomes more sophisticated in order to more closely conform to reality, the associated data requirements increase. A point exists at which the benefits of a more realistic mathematical model are outweighed by the difficulty and expense of collecting the data necessary to adequately define such a model.

The available techniques and equipment may limit the results which can be obtained from a practical mathematical model. In the case of mathematical modeling, available numerical solution schemes and computer equipment may not permit the economic solution of a modeling problem even though the basic mathematics describing the system can be formulated.

Related to both the data requirements and the available mathematical tools are the simplifications which are always applied in modeling a complex situation such as the Hanford groundwater system. Some of the simplifications are automatic and perhaps even trivial; such as, the assumption that the Columbia River will not change course to a significant degree throughout a simulation period. Other simplifications are

not trivial and may be critical to the success of the mathematical modeling effort. Among the simplifications which have been applied to the Hanford flow system in the past is the Dupuit-Forchheimer or Boussinesq approximation.^[5] The important advantage gained by applying this approximation is that the flow system can be treated as being two-dimensional rather than three-dimensional thus reducing the number of unknowns in the equations and also the data requirements. In using this approximation the assumption is made that the equipotential surfaces are vertical and the flow is essentially horizontal. It has been common practice at Hanford to also assume that discharges to the radioactive waste ponds are immediately transmitted to the water table without consideration of phenomena occurring within the partially saturated zone. These basic assumptions could be eliminated by the application of an appropriate multiphase, three-dimensional model.

Any model of the Hanford subsurface system will have a defined set of boundaries within which lie the system and outside of which lie the rest of the world. The location and nature of the boundaries depend upon the conceptual description being treated. If, for example, no interaction between the intermediate-local waste discharge flow regime and the underlying regional flow system were considered, a limited predictive model would be constructed which would not include any part of the regional system.

Once a model has been constructed to adequately reflect the conceptual description, the time dependent conditions of the system require examination. Such time dependent conditions involve water fluxes across the boundaries or migration of radionuclides within the system. They can be the result of natural conditions, waste management decisions, or other artificial conditions such as the dynamic river elevation patterns created by the dams constructed along the Columbia River System.

The process of applying modeling to achieve management goals follows a definite pattern. The sequence of events which occur in

mathematically modeling the Hanford groundwater system can best be illustrated as in Figure 5. Very often in groundwater modeling the phenomena associated strictly with flow can be considered separately from the chemical reaction-solute transport phenomena. This is true because in most situations of interest the chemical reaction-transport processes do not significantly affect the flow patterns. The reverse is not true since flow has a major impact upon contaminant transport.

The data requirements needed for both the flow models and the contaminant transport models are outlined in Figure 6. Specific requirements will vary depending on the type of mathematical model and the desired precision of the model output. Table 1 outlines the type of data needed and the sources that can be used in obtaining the data. As noted in Table 1 the type of data depends on the model characteristics. The categories of mathematical models listed in Table 1 include all the model types applicable to the Hanford groundwater regime. Each category is discussed in the following section.

FIGURE 5
MODELING FRAMEWORK

FIGURE 6
DATA REQUIREMENTS

TABLE 1
GENERAL DATA REQUIREMENTS

Data/Parameter Type	Data Source	Flow Model Category		
		Saturated Data Requirements	2 and 3-D, Multiphase Data Requirements	Partially Saturated Data Requirements
Hydraulic Conductivity	lithologic data, pump tests, laboratory measurements	wide coverage needed; data density depends on heterogeneity of the sediments	same as for Saturated case	dense coverage needed in the area of expected flow
Effective Porosity	laboratory measurements, lithologic data, electrical conductivity of fluid filling the void spaces	wide coverage, the needed data density related to the heterogeneity and packing of the sediments	same as for the saturated case; vertical component also needed for 3-D	dense coverage needed in the area of expected flow
Vertical Compressibility of the Solid Skeleton	lithologic data, laboratory measurements	generally a low data density is needed, may become more important in deep, confined aquifers	same as for the saturated case	same as for the saturated case
Soil Moisture Characteristics (capillary pressure, % saturation, relative permeability)	laboratory studies, lithologic data	not applicable	dense coverage needed only in the partially saturated zones of interest	dense coverage needed in the area of expected flow
Leakage	geologic and lithologic data, potential measurements, pump tests, tracer movement, water mass balance	good coverage in areas where potential measurements show possible leakage	same as for the saturated case	not applicable
Fluid Density, Compressibility, and Viscosity	laboratory measurements; calculated from pressure, temperature, and solute concentration measurements	generally considered constant	generally considered constant	generally considered constant
Recharge and Discharge Locations and Rates	pump tests, geologic studies, flow measurements for man-made recharge/discharge, potential measurements	good data needed for all significant sources	good data needed for all significant sources	good data needed for all significant sources
Time Varying Potentials Along the Boundaries	potential measurements, measurements of surface water elevations along the boundaries	quality and density of data related to the anticipated range	same as for the saturated model	not usually applicable at Hanford
Geometric Description of Aquifer Boundaries	lithologic data, geologic data, potential measurements	wide coverage needed, especially in areas of rapid change	wide coverage needed, especially in areas of rapid change of the saturated zone	not usually applicable
Initial Potential Distribution	field measurements at wells or piezometers	wide coverage needed; dense coverage in areas of rapid change is desirable	same as for the saturated model	good coverage for area of expected flow
Transport-Reaction Model Category				
Data Requirements				
Dispersion Coefficients	laboratory measurements, tracer tests, correlations with lithologic data	relatively low data density compared to parameters such as hydraulic conductivity is usually needed, data coverage should be wide enough to cover the area of expected contaminant migration		
Sorption Coefficients	laboratory measurements, correlations with lithologic data	dense coverage in the areas of contaminant disposal and less dense elsewhere, data density also depends upon characteristics of the wastes		
Radioactive Decay Rates	laboratory measurement	the half-lives of all radionuclides of interest at Hanford have been determined, uncertainties exist only when the distribution of the radionuclides in a waste stream or groundwater system are unknown		
Chemical Reaction Constants	laboratory measurements, correlations with lithologic data	dense coverage in the areas of contaminant disposal and less dense elsewhere, data density also depends upon the characteristics of the wastes		
Contaminant Initial Locations	field sampling	wide coverage needed, high data density in areas of waste disposal and less dense elsewhere		
Contaminant Initial Concentrations	field sampling	wide coverage needed, high data density in areas of waste disposal and less dense elsewhere		
Contaminant Concentrations of Recharge and Discharge Sources	sampling of waste disposal streams, calculation from plant production data	all waste streams with significant contaminant concentrations should be periodically sampled and the samples analyzed		

MATHEMATICAL MODELS

As previously mentioned, any realistic modeling effort requires some sort of simplifying assumptions to bridge the gap between reality, our current understanding of the actual system, and practicability. Certain basic assumptions are generally agreed upon and accepted, whereas others require justification based on data and observations made on the actual system being modeled. In any of the equations that we will write in this section, one large step of modeling effort and a large set of assumptions has been removed. We are referring to the arguments discussed in "Dynamics Of Fluids in Porous Media" by Jacob Bear,^[6] which takes us from the complex world of porous media particles and the associated tortuous flowpaths to the regime of representative elementary volumes (REV) and the fluid flow continuum. These assumptions are generally accepted and are complex enough that they will not be presented here.

As indicated earlier, the groundwater system at Hanford generally allows the flow modeling problem to be considered separately from the chemical reaction-solute transport problem. This separation of flow from transport is based upon the assumption that the movement and transport of wastes through the porous soil matrix does not cause any significant changes in the hydraulic properties of the soil. The only exception to note to this situation is the case of a waste storage tank leaking thermally and radioactively hot liquid which is also chemically caustic. In the local region (within a few meters) beneath and around the leaking tank, temperature and chemical reaction induced flow modifications are considered important. The case of a leaking radioactive waste storage tank is an extremely difficult and complex modeling problem. A great deal is still unknown regarding the chemical reactions between the caustic, viscous, hot, highly radioactive waste stored in tanks and the various types of soils. Work in this area is underway.

Observations of temperatures in the regional aquifer systems underlying Hanford do not reveal large enough temperature variations to warrant inclusion of temperature dependent driving forces in the equations developed for describing the flow continuum. In the flow equations developed in the following pages, only the isothermal and transport independent equations will be discussed and thus, the flow and transport equations can be handled separately. The flow field that is computed for the fluid may be used in a Lagrangian sense in solving the transport problem. Figure 7 illustrates the fluid flow mechanisms and equation formulations which will be discussed. Figure 8 illustrates the contaminant transport mechanisms which will be discussed.

From the description of the flow system presented in the preceding sections and illustrated in Figure 4, it is clear that the most representative formulation of this subsurface fluid flow system would be a fully three-dimensional dynamic air and water flow system.

GENERAL MODEL ASSUMPTIONS

The general assumptions made in mathematically modeling the Hanford groundwater system are that:

- the fluid and porous material form a continuous system,
- the smallest unit of analysis called the Representative Elementary Volume (REV) is of such a size that specification of constant values of its various parameters (porosity, permeability, etc.) does not introduce significant errors,
- the flow regime is laminar,
- the network of channels connected to each other by junctions produces average gradients of pressure, density, viscosity, and solute concentration in any REV that includes a sufficiently large number of channels and junctions,

FLUID FLOW	SATURATED			PARTIALLY SATURATED (STABLE AIR, DYNAMIC WATER PHASE)	MULTIPHASE (DYNAMIC GAS AND WATER FLOW)
DIMENSIONS	CONFINED AQUIFER	UNCONFINED AQUIFER (FREE SURFACE REPRESENTATION)	BOUSSINESQ APPROXIMATION		
1D					
2D					
3D					
2D MULTILAYERED

Does Not Apply
To Hanford

FIGURE 7

FLUID FLOW EQUATION FORMULATIONS TO BE DISCUSSED

CONTAMINANT TRANSPORT			
CONSERVATIVE CONSTITUENTS		REACTIVE CONSTITUENTS	
Advective Changes Only	Advective and Dispersive Induced Changes	ADVECTIVE AND DISPERSIVE CHANGES WITH:	
		Equilibrium Reactions	Kinetic Reactions

FIGURE 8

TYPE OF TRANSPORT EQUATION FORMULATIONS TO BE DISCUSSED

- all average gradients are independent of the geometric shape of a single channel within an REV,
- temperature variations in the system are small enough that temperature dependent driving forces can be ignored, and that
- the transport of chemical and radioactive wastes through a porous medium does not cause any significant changes in the porous material, thus altering its fluid flow parameters.

With the above assumptions in mind, the most general case we will consider is that of two dynamic immiscible fluids (air and water which contain chemical and radioactive wastes) in an isothermal, porous medium, three-dimensional flow system. The complete development of these equations and associated assumptions is covered in great detail in "Dynamics of Fluids in Porous Media" by Jacob Bear.^[6] The development given here will necessarily be limited, yet of sufficient detail to illustrate the basic assumptions and shortcomings.

FLOW OF IMMISCIBLE FLUIDS (MULTIPHASE FLOW)

Pressure and Saturation

In the case of simultaneous flow of two immiscible fluids or phases, such as air and water in a porous media domain, the interfacial tension between the two fluids is nonzero and a distinct fluid(air)-fluid(water) interface separates the fluids within the pore space and a capillary pressure difference, P_c , exists across the interface at each point on it. Figure 9 illustrates the porous medium, the wetting (water) and nonwetting (air) phases and their associated pressures, P_2 and P_1 . When the voids in the porous medium are filled by two immiscible fluids, as indicated in Figure 9, the saturation at a point with respect to a particular fluid is defined as the fraction of the void volume of the porous medium occupied by the fluid within a Representative Elementary Volume (REV) at that point in the medium. Thus,

FIGURE 9

DIAGRAM OF A POROUS MEDIUM WITH TWO IMMISCIBLE FLUIDS

$$S_{\alpha} = \frac{\text{volume of fluid } \alpha \text{ within an REV}}{\text{volume of voids within an REV}} \text{ (dimensionless)}$$

$$\sum_{\alpha=1}^2 S_{\alpha} = 1.0$$

where

$\alpha=1$ =air (nonwetting)

$\alpha=2$ =water (wetting), and

$$P_c = P_c(S_2) \quad [ML^{-1}T^{-2}]$$

where P_c is an empirical function of S_2 .

Development of an analytic relationship between P_c and S_2 for a realistic porous medium cannot be accomplished. Laboratory experiments are the only way to derive this relationship for any given porous medium.

Among the phenomena worth mentioning at this point are the irreducible wetting fluid saturation (S_{o2}) and the irreducible nonwetting fluid saturation (S_{o1}). S_{o2} is the limit below which further reduction in water content cannot be accomplished by a simple displacement mechanism. Further reduction could only occur via some other mechanism such as evaporation, which could result by flowing dry air through the soil matrix. Since we are considering an isothermal system, this phenomenon is beyond the realm of interest. S_{o1} is the limit above which further increases in the water content (or below which further reductions in air content) cannot be accomplished because a certain amount of residual air is trapped. A typical capillary pressure versus saturation curve is shown in Figure 10. The solid line represents the drainage (decreasing water content) and imbibition (increasing water content) curves which in the ideal case are the same curve. A phenomenon which appears to be more pronounced in the laboratory than in the field^[7] can be illustrated by the dashed imbibition curve shown on

V7606-8.2

FIGURE 10

IDEALIZED GRAPH OF CAPILLARY PRESSURE, P_c ,
VERSUS S_1 AND S_2 SHOWING THE HYSTERESIS PHENOMENA

Figure 10. This phenomenon, known as hysteresis, comes about as a result of slight differences in the P_c versus S_2 curve related to the past history of the porous medium and whether S_2 is increasing or decreasing. Although hysteresis is mentioned for completeness, its importance in Hanford field problems is expected to be small. It will be included in Hanford multiphase modeling only if evidence becomes available which indicates such a need.

As mentioned previously, the relationship between capillary pressure and saturation can only be determined for natural porous media via laboratory experiments, and this relationship represents one of the parameters which must be determined.

Equations of Motion

The equations of motion are developed from the following view of the physical system which is based upon experimental evidence. When two immiscible fluids flow simultaneously through a porous medium, each fluid establishes its own tortuous paths, which form very stable channels and a unique set of channels is assumed to correspond to every degree of saturation.

Darcy's law originally developed for single phase saturated flow has been experimentally verified as extendable to two phase flow for immiscible fluids.^[6] The resulting equations of motion for an anisotropic heterogeneous porous medium are:

$$q_{i1} = - \frac{k_{ij1}}{\mu_1} \left(\frac{\partial P_1}{\partial x_j} + \rho_1 g \frac{\partial z}{\partial x_j} \right) \quad (1)$$

$$q_{i2} = - \frac{k_{ij2}}{\mu_2} \left(\frac{\partial P_2}{\partial x_j} + \rho_2 g \frac{\partial z}{\partial x_j} \right) \quad (2)$$

where:

q = volume flux per unit area [LT^{-1}]

i, j = cartesian coordinate indices

= 1, 2, 3;

$k_{ij\alpha}$ = second rank tensor components of effective permeability to component α at saturation S_α [L^2]

α = 1, 2; 1 = air; 2 = water

μ_α = viscosity of fluid α at pressure P_α [$ML^{-1} T^{-1}$]

P_α = pressure of fluid α [$ML^{-1} T^{-2}$]

ρ_α = density of fluid α at pressure P_α [ML^{-3}]

g = acceleration of gravity [LT^{-2}]

The discussion on conceptual modeling brought out the fact that the Hanford system is heterogeneous. The degree of true anisotropy has not been established but may be of much less importance than the heterogeneity. Until such time as true anisotropy has been demonstrated to be an important factor in the Hanford groundwater system it will not be included in the modeling process. This does not mean that anisotropy will be ignored; some elements of anisotropy or apparent anisotropy will be included in the formulation of the final versions of Hanford groundwater flow codes if such are needed. There are no groundwater flow codes available anywhere which treat the completely general case of true anisotropy. Further discussion of the detailed mathematical models will assume an isotropic porous medium. The assumption of isotropy results in the effective permeability tensors reducing to scalars and equations (1) and (2) become

$$\bar{q}_\alpha = - \frac{k_\alpha}{\mu_\alpha} \nabla (P_\alpha + \rho_\alpha g z) \quad (3)$$

where ∇ is the gradient operator $= \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$

Relative Permeability - Permeability

It is typical to define the k_1 and k_2 in terms of k and k_{r1} and k_{r2} where k is the intrinsic permeability of the medium to a single phase fluid completely saturating it and k_{r1} and k_{r2} are the relative permeabilities of the medium (functions of saturation S_1 and S_2) to fluid 1 and fluid 2. At any level of saturation, S_α , the $k_{r\alpha}$ are determined by the following ratio:

$$k_{r\alpha} = \frac{k_\alpha}{k}.$$

It is difficult to derive the $k_{r\alpha}$ except through idealized porous medium models or through experiments. The k is usually determined for the porous medium and some saturating fluid and then the $k_{r\alpha}$ can be determined as a function of saturation S_α . The $k_{r\alpha}$ may also be calculated from the S versus P_c curves. Typical functions of $k_{r\alpha}$ can be determined as a function of S_α for air and water in consolidated sand (Figure 11). In our air-water system as $S_1 \rightarrow S_{o1}$, as shown in Figure 11, the channels of the nonwetting fluid begin to break down and at $S_1 = S_{o1}$, the flow channels for the air become completely discontinuous, the effective permeability to air becomes zero and the air movement ceases. The remaining air is entrapped. Similarly, as $S_2 \rightarrow S_{o1}$, the water flow channels break down and at $S_2 = S_{o1}$ they are completely discontinuous causing the effective permeability for water to become zero and the water flow to cease. We have assumed that the $k_{r\alpha}$ are independent of pressure gradients and viscosity differences between the two phases. Although there have been studies which indicate this is not strictly true, the concept of a relative permeability that depends only on saturation appears to be a good approximation for all practical purposes.^[6]

Conservation of Mass

In our subsurface flow system, we assume conservation of mass such that

V7606-8.1

FIGURE 11

TYPICAL RELATIVE PERMEABILITIES OF GAS (1)
AND WATER (2) FOR UNCONSOLIDATED SAND AS A
FUNCTION OF SATURATION

$$\frac{\partial(nS_{\alpha}\rho_{\alpha})}{\partial t} + \nabla \cdot (\rho_{\alpha} \bar{q}_{\alpha}) - Q_{\alpha} = 0 \quad (4)$$

where:

n = porosity of solid medium (dimensionless)

S_{α} and ρ_{α} as defined earlier

Q_{α} = source or sink function [$ML^{-3}T^{-1}$]

$\bar{q}_{\alpha}$ = vector of average discharge velocities from the equations of motion [LT^{-1}]

$\alpha = 1, 2$ (1 = air; 2 = water)

Within each Representative Elementary Volume (REV) the increase or decrease in mass of component α is a function of the algebraic sum of flows into and out of the REV from the surrounding continuum plus the amount added or withdrawn from some external source.

System of Multiphase Flow Equations

In two phase (air-water), three-dimensional, isotropic, heterogeneous fluid flow there are 13 dependent variables which we have discussed and they are as follows:

<u>Variable Description</u>		<u>Number of Variables</u>	
Volumetric flux	$\bar{q}_1, \bar{q}_2$	2	one for each phase
Saturation	S_1, S_2	2	one for each phase
Density	ρ_1, ρ_2	2	one for each phase
Viscosity	μ_1, μ_2	2	one for each phase
Relative permeability	k_{r1}, k_{r2}	2	one for each phase
Pressure	P_1, P_2	2	one for each phase
Capillary pressure	P_c	<u>1</u>	
Total		13	

Hence, we need 13 equations to derive a complete solution of the flow (velocity, pressure and saturation distributions within the flow domain and their time variations) and the fluids (density and viscosity as a function of position and time). The independent variables are time, t , and the spatial variables x, y, z .

The following are the equations for multiphase flow of two immiscible compressible fluids in a heterogeneous isotropic porous medium:

- Two equations of motion

$$\bar{q}_\alpha = -k \frac{k_{r\alpha}}{\mu_\alpha} \nabla (P_\alpha + \rho_\alpha g z) \quad (5-6)$$

$$\alpha = 1, 2$$

- Two equations of continuity

$$\frac{\partial (n S_\alpha \rho_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha \bar{q}_\alpha) - Q_\alpha = 0 \quad (7-8)$$

$$\alpha = 1, 2$$

- Saturation equation

$$\sum_{\alpha=1}^2 S_\alpha = 1.0 \quad (9)$$

- Two equations of state for density

$$\rho_\alpha = \rho_\alpha (P_\alpha) \quad (10-11)$$

$$\alpha = 1, 2$$

- Two equations of state for viscosity

$$\mu_\alpha = \mu_\alpha (P_\alpha) \quad (12-13)$$

$$\alpha = 1, 2$$

- Two equations of relative permeability versus fluid saturations

$$k_{r\alpha} = k_{r\alpha} (S_\alpha) \quad (14-15)$$

$$\alpha = 1, 2$$

- Relationship between P_1 , P_2 , and P_c

$$P_c = P_c (S_2) \quad (16)$$

$$P_c = P_1 - P_2 \quad (17)$$

Simplified Multiphase Three-Dimensional Flow Equations

The set of necessary equations can be simplified by eliminating the dependent variables, $\bar{q}_\alpha$, by inserting the equations of motion into the continuity equation and making the simplifying assumptions that water is incompressible and that the porous medium is nondeformable. Thus,

$$n \frac{\partial(S_1 \rho_1)}{\partial t} + \nabla \cdot \left[\rho_1 k \frac{k_{r1}}{\mu_1} \nabla (P_1 + \rho_1 g z) \right] - Q_1 = 0 \quad (18)$$

$$n \frac{\partial(S_2)}{\partial t} + \nabla \cdot \left[k \frac{k_{r2}}{\mu_2} \nabla (P_2 + \rho_2 g z) \right] - \frac{Q_2}{\rho_2} = 0 \quad (19)$$

The equations of state and other applicable relationships (see Equations 9-17) given the two assumptions above are:

$$S_1 + S_2 = 1$$

$$P_c = P_c (S_2)$$

$$P_c (S_2) = P_1 - P_2$$

$$\mu_1 = \mu_1 (\rho_1)$$

$$\rho_1 = \rho_1 (P_1)$$

$$k_{r1} = k_{r1} (S_1)$$

$$k_{r2} = k_{r2} (S_2)$$

subscript 1 = air, 2 = water

Assumptions

The assumptions associated with multiphase flow in addition to those mentioned under general model assumptions are:

- the fluids (air-water) are immiscible and the interfacial tension between the two fluids is nonzero and a distinct fluid-fluid interface separates the fluids within the pore space of the REV;
- the capillary pressure P_c can be expressed as a single valued function of saturation alone as previously discussed;
- when two immiscible fluids flow simultaneously through a porous medium, each fluid establishes its own tortuous flow-paths, which form very stable flow channels and there is a unique set of these channels for each degree of saturation;
- the relative permeability functions are functions only of the saturation (i.e., pressure gradients and viscosity differences do not alter the medium's relative permeability scalar);
- conservation of mass is assumed;
- the porous medium is isotropic, heterogeneous, and nondeformable;
- the water is incompressible; and
- density and viscosity of the air can change as a function of pressure.

Boundary and Initial Conditions

In addition to the equations and physical properties discussed above, boundary conditions along with initial conditions are also required. Boundary conditions include:

- A geometrical description of the physical boundaries of the region within which the equations are to be solved.
- At these geometrical boundaries, a description of what kind of boundary:
 - recharge, inflow, or outflow boundary (flow across boundary is known);

- no flow boundary (like might occur at a basalt outcrop);
- values for a sufficient set of dependent variables are known (i.e., a held boundary such as might occur along the Columbia River).

When a transient solution to the problem is desired, then the boundary conditions must be specified for all times within the period of interest.

Without defining a particular problem, it is somewhat difficult to make a complete list of what must be specified along a boundary, but the conditions specified at the boundary must be consistent with the modeler's interpretation of what is happening in the real world; as well as with the equations above. For example, if along some boundary of the region you know the pressures, P_α , then you cannot also specify the q_α or P_c or μ_α or ρ_α or S_α since they are uniquely determined from the equations and initial conditions once the P_α are specified.

Typically, the boundary conditions that would be supplied, in addition to the geometric description, would be one of the following sets of data at each point along the boundary:

- P_1 and P_2
- P_1 or 2 and P_c
- P_1 or 2 and $\frac{\partial(P_1 \text{ or } 2 + \rho_1 \text{ or } 2 \text{ } gz)}{\partial X_i} = 0$ for a given direction X_i
- P_1 or 2 and q_2 or 1
- $q_\alpha \quad \alpha = 1, 2$

The initial conditions define the initial values of the dependent variables everywhere within the region being modeled. Because of the relationships between the dependent variables, a description of the

initial values P_1 and P_2 would be sufficient to determine the entire set of dependent variables. Other sufficient sets include:

- P_1 or P_2 and P_c
- P_α

Results Obtainable

A solution to the three-dimensional multiphase flow equations described with the associated boundary conditions would yield the air and water pressures (or potentials) throughout the three-dimensional space of the system being modeled as a function of time (for transient case). From this, the three-dimensional air and water flow fields and position of the phreatic surface can be calculated.

Limitations

The limitations of the multiphase model include the amount of data required to adequately define the model and the computer resources which must be applied to any but the smallest regions. Perhaps more basic however is the limited need to describe the air phase flow field.

Dimensionality

By eliminating one coordinate axis from the three-dimensional model, a two-dimensional multiphase model may be applied in either a horizontal (xy) slab, a vertical (xz) slab, or a cylinder (rz). In such applications the " ∇ " operation would be defined as $\frac{\partial}{\partial x} + \frac{\partial}{\partial y}$, $\frac{\partial}{\partial x} + \frac{\partial}{\partial z}$, or $\frac{\partial}{\partial r} + \frac{\partial}{\partial z}$ respectively.

The required boundary conditions and results obtainable would also be expressed in terms of two dimensions. Although a one-dimensional multiphase model is conceivable, field applications appear to be very limited. A one-dimensional model may have application in laboratory column experiments.

Applications

Full utilization of a multiphase model at Hanford would involve situations where both a dynamic air phase and a dynamic water phase are important. Such an application may exist where air is being injected into the subsurface to control the movement of contaminated water. An appropriate multiphase model would also apply to situations where only one of the phases is dynamic or to continuous systems involving zones of multiphase flow and zones of single phase (saturated) flow. Since the partially saturated model (detailed treatment to follow) is a subset of the multiphase flow model, any problem to which a partially saturated model applies could be solved at least as well (but perhaps at a higher computer cost) by the multiphase model.

PARTIALLY SATURATED FLOW

The discussion to this point has been directed towards the situation where both air and water phases are dynamic. Now we will treat the case of a static air phase often referred to as "partially saturated" or "unsaturated" flow.

The assumption of a completely static air phase means that P_1 is everywhere constant (P_1 = atmospheric pressure which we will define as a reference pressure of zero), there are no air source/sink terms ($Q_1 = 0$), and no air flow (neglecting gravity effects of the air). Thus equation (18) becomes identically zero. Replacing

$\frac{k_r k_{r2}}{\mu^2}$ of equation (19) by $K(S_2) [M^{-1} L^3 T]$ the general equation for partially saturated flow becomes

$$n \frac{\partial(S_2)}{\partial t} + \nabla \cdot [K(S_2) \nabla (P_2 + \rho_2 g z)] - Q_2 / \rho_2 = 0 \quad (20)$$

$$\text{and } P_c(S_2) = -P_2$$

Since we are dealing only with the water phase equation the subscript $\alpha = 2$ will be dropped at this point. Expanding equation (20) yields

$$-n \frac{dS}{dP} \frac{\partial P}{\partial t} + K \nabla^2 P + \nabla K \cdot \nabla P - \frac{dK}{dS} \frac{dS}{dP} [\nabla P \cdot \nabla P + \rho g \frac{\partial P}{\partial z}] + \rho g \frac{\partial K}{\partial z} - \frac{Q}{\rho} = 0 \quad (21)$$

which is the expanded form for partially saturated flow in heterogeneous, isotropic material. Eliminating the terms in equation (21) which deal with heterogeneity leaves:

$$-n \frac{dS}{dP} \frac{\partial P}{\partial t} + K \nabla^2 P - \frac{dK}{dS} \frac{dS}{dP} [\nabla P \cdot \nabla P + \rho g \frac{\partial P}{\partial z}] - \frac{Q}{\rho} = 0 \quad (22)$$

$$(\nabla K = 0, \frac{\partial K}{\partial z} = 0)$$

which is the expanded equation for partially saturated flow in homogeneous, isotropic material. Elimination of the partially saturated terms from equation (21) leaves

$$K \nabla^2 P + \nabla K \cdot \nabla P + \rho g \frac{\partial K}{\partial z} - \frac{Q}{\rho} = 0 \quad (23)$$

which is the equation for saturated flow in heterogeneous, isotropic material. Often in such systems it is more convenient to use a potential formulation which is easily obtained by defining a potential $\Phi = P + \rho g z$ and then equation (23) becomes the more widely used form:

$$K \nabla^2 \Phi + \nabla K \cdot \nabla \Phi - \frac{Q}{\rho} = 0. \quad (24)$$

Finally, if the terms related to heterogeneity are dropped from equation (24) we have

$$\nabla^2 \Phi - \frac{Q}{K \rho} = 0 \quad (25)$$

which is the equation for saturated flow in a homogeneous, isotropic medium with a source/sink term.

The purpose of the above mathematical exercise starting with the expansion of equation (20) is to illustrate the general application of equation (21) to a continuous system involving zones of partial saturation, full saturation, homogeneous medium and heterogeneous media.

Assumptions

In addition to the assumptions presented under general model assumptions and multiphase fluid flow, the following apply:

- the air phase is completely static (the air pressure is constant), and
- gravity effects of the air are neglected.

Boundary and Initial Conditions

The requirements for the boundary and initial conditions for unsaturated flow are similar to those for multiphase flow except that only the water pressure (or potential) is needed for the situations specified in multi-phase flow as requiring P_1 or P_2 and P_c or P_α , since for the partially saturated case P_1 is equal to atmospheric pressure or a gage pressure of zero and $P_2 = P = -P_c$. Quite often the boundary conditions will be measured as the potential, Φ instead of the water pressure, P , in which case a vertical reference datum must also be specified.

Results Obtainable

A solution of the partially saturated flow equation with associated boundary conditions would yield the water pressures or potentials throughout the system as a function of time. This would allow a determination of the water flow field in space and the position of the free surface.

Limitations

The three-dimensional, partially saturated flow model will not yield the air phase flow (if it is important) but requires less data and less computer resources (fewer equations to solve) than the multiphase flow model.

Dimensionality

The dimensionality discussion under multiphase flow is applicable to partially saturated flow except that only the liquid equation is considered.

Applications

As the development of the equations show, the partially saturated model category may include zones of partial saturation and zones of full saturation. Thus, the applications include such problems as partially saturated flow, location of the phreatic surface between partially saturated and saturated zones, and flow within the saturated zone. An attractive feature of this type of model similar to that of the multiphase flow model is the capability of treating the partially saturated and saturated zones as a continuous system. In the treatment of a discharge pond, for example, the flow within the partially saturated zone between the pond bottom and the water table and the flow (including significant vertical components) within the saturated zone near the pond could be handled as a continuous problem by an appropriate three-dimensional partially saturated code. The changing position and shape of the water table (phreatic) surface would also be predictable with a partially saturated model given the validity of the static air phase assumption.

SATURATED, CONFINED FLOW

Saturated porous medium flow bounded both above and below by impermeable boundaries is said to occur in a pressurized or confined

aquifer. Equations 23 and 24 developed under the partially saturated flow treatment apply to saturated, confined flow.

Assumptions

In addition to the general assumptions, the assumptions which apply to confined, saturated liquid flow as presented are:

- the porous medium is isotropic, heterogeneous and nondeformable,
- conservation of mass is assumed,
- the liquid is incompressible,
- the system is everywhere saturated with liquid at all times, and
- the flow system is confined so that the upper and lower boundaries are fixed both in space and time.

Boundary and Initial Conditions

Specification of the potential or pressure distributions or fluxes at the flow boundaries (or "ends") of the aquifer system is required. The confining layers are described by assigning zero fluxes across such boundaries. The definition of the potential (or pressure) distribution throughout the system at the initial time constitutes the required initial condition.

Results Obtainable

Solution of the saturated flow equation and associated boundary conditions yields the liquid potentials (or pressures) throughout the confined system as a function of time. The potential distribution combined with the hydraulic conductivity and porosity distributions also permits determination of the liquid velocity field if desired.

Limitations

The combination of equations and boundary conditions associated with this section is limited to saturated flow in a confined aquifer system.

Dimensionality

The saturated, confined flow model may be readily applied in two dimensions to a vertical slab (xz) or cylinder (rz). The principal assumption for such cases is that the flow in the lateral or "y" direction for an xz slab or the direction perpendicular to the radii in the rz cylinder is negligible. For such cases the "∇" in equations 24 and 25 would be defined as

$$\frac{\partial}{\partial x} + \frac{\partial}{\partial z} \text{ or } \frac{\partial}{\partial r} + \frac{\partial}{\partial z}$$

respectively. The boundary conditions are specified in only two dimensions and the model results are expressed in only two dimensions. The two-dimensional horizontal slab (xy) is treated under Boussinesq Flow Model description. A one-dimensional, confined flow model is conceivable but of very limited field application at Hanford.

Applications

This type of model may be applied to aquifer systems that are known to be confined throughout the region of interest.

SATURATED, UNCONFINED OR FREE SURFACE FLOW MODEL

Unconfined or free surface flow in a saturated system arises when there is no upper confining layer. Under these conditions the upper boundary of the system is the interface between the saturated and partially saturated zones which is usually referred to as the water table. Unlike confined flow, the location of the upper boundary is not fixed but may vary with position and time and is unknown beforehand.

The equation for saturated, heterogeneous flow expressed in terms of the potential, Φ , as developed under the partially saturated flow model is

$$K \nabla^2 \Phi + \nabla K \cdot \nabla \Phi - \frac{Q}{\rho} = 0 \quad (24)$$

The mathematical difference between the confined aquifer case and the unconfined situation arises from the necessity of solving for the free surface boundary as part of the potential distribution. Accretion in an unconfined aquifer may be considered as part of the free surface boundary condition. The Q/ρ term of Equation 22 is now limited to source/sinks which occur below the free surface such as from wells.

The free surface boundary may be described by some function $F(x,y,z,t)$ where $F(x,y,z,t) = \Phi(x,y,z,t) - z = 0$.

Continuity considerations require that

$$\bar{V} = \frac{1}{n_e} (\bar{q} - \bar{N})$$

where

$\bar{V}$ = is the velocity of the water particles belonging to the free surface [LT^{-1}],

n_e = is the effective porosity of the soil matrix [dimensionless],

$\bar{q}$ = is the specific discharge [LT^{-1}], and

$\bar{N}$ = is the accretion [LT^{-1}].

In order to describe the time rate of change in the position of the free surface described by $F(x,y,z,t)$ in a Lagrangian sense (coordinate system moving with the flow field) the substantial derivative of the function F defining the free surface is obtained which is

$$\frac{DF}{Dt} = \frac{\partial F}{\partial t} + \bar{V} \cdot \nabla F = 0. \quad (26)$$

For an isotropic medium $q = -K \nabla \Phi$ and substituting for F and $\bar{V}$ into equation (26) with appropriate vector manipulation results in

$$n_e \frac{\partial \Phi}{\partial t} - K(\nabla \Phi)^2 + \frac{\partial \Phi}{\partial z} (K + N) - N = 0 \quad (27)$$

which is the general equation for the free surface boundary in an unconfined flow system. This equation is nonlinear with respect to Φ . A linear approximation to equation 27 may be obtained by removing the second term which yields

$$n_e \frac{\partial \Phi}{\partial t} + \frac{\partial \Phi}{\partial z} (K + N) - N = 0 \quad (28)$$

A rigorous, simulation of the free surface, saturated flow system requires simultaneous solution of equations 24 and 27. An approximation of such flow may be obtained by the simultaneous solution of equations 24 and 28.

Assumptions

In addition to the general model assumptions, the assumptions of the saturated, free surface model described in this section are the same as those for saturated, confined flow except that

the upper boundary of the system is assumed to be a sharp liquid interface between the saturated and partially saturated zones. This interface is movable and its position with time forms part of the required solution.

Boundary and Initial Conditions

The boundaries of an unconfined aquifer (other than the free surface boundary) must be described by a set of potentials, pressures, or fluxes. The required initial condition is the potential or pressure distribution throughout the system.

Results Obtainable

The solution of the saturated, unconfined flow model described above yields predictions of potentials throughout an unconfined or combination confined/unconfined system as well as the position of the free surface. As in confined flow the potential distribution combined

with the hydraulic conductivity and porosity distributions permits determination of the velocity field which is required for transport modeling.

Limitations

Rigorous solution of the nonlinear, free surface boundary condition simultaneously with the saturated flow equation is quite difficult and requires considerable computer resources.

Rather than solve the free surface boundary condition equation an approach used in at least one unconfined aquifer flow model involves substituting the upper grid block free surface height, Δh , as measured from the bottom of the block for the block depth Δz in calculating the block transmissivity (hydraulic conductivity times depth). The Δh from a previous calculation is used so that a relatively small time step or an iterative technique is required.^[8] In another iterative approach to the free surface boundary problem the flow velocity normal to the free surface is calculated and the position of the free surface is determined at the new time step.^[9]

Dimensionality

The dimensionality discussion under the saturated confined flow model is applicable to saturated, unconfined flow. Again, the horizontal slab (xy model) is treated under the Boussinesq flow model description. A one-dimensional, free surface model is of little value.

Applications

The solution of free surface flow problems with significant vertical flow components appears practical. If the soil moisture characteristics are known, a multiphase type flow model would yield more accurate estimates of both the saturated potentials and phreatic surface position as well as giving the partially saturated zone potentials. In practice,

the saturated unconfined system flow model (perhaps with one of the iterative techniques for determining the free surface discussed above) appears to be more practical than a multiphase type model for obtaining useful estimates of saturated zone potentials over large areas.

BOUSSINESQ TYPE FLOW

Previous discussion has shown that the free-surface saturated flow problem is difficult to solve exactly because of the nonlinear free-surface boundary condition. Often an exact solution of the general, three-dimensional, saturated flow equation and free-surface boundary condition is not required to obtain useful results. The Dupuit-Forchheimer or Boussinesq approximate method assumes a simplified, two-dimensional horizontal view of the groundwater system which allows the free-surface boundary condition and the flow equation to be combined into a single equation amenable to practical solution techniques. For simplicity sake we will refer to this method as the Boussinesq flow model.

Let x, y, z be the coordinates of a fluid particle, then dx/dt , dy/dt and dz/dt are the components of "pore velocity," and the Darcian seepage velocities are:

$$V_x = n_e \frac{dx}{dt} \quad (29)$$

$$V_y = n_e \frac{dy}{dt} \quad (30)$$

$$V_z = n_e \frac{dz}{dt} \quad (31)$$

Now if we let $z = h(x, y, t)$ represent the coordinate of the free surface and formally differentiate with respect to time, we have:

$$\frac{\partial z}{\partial t} = \frac{\partial h}{\partial x} \frac{dx}{dt} + \frac{\partial h}{\partial y} \frac{dy}{dt} + \frac{\partial h}{\partial t} \quad (32)$$

Substituting the Darcian velocities and rearranging we have:

$$n_e \frac{\partial h}{\partial t} + V_x \frac{\partial h}{\partial x} + V_y \frac{\partial h}{\partial y} - V_z = 0 \quad (33)$$

The Dupuit assumptions used in this model may be simply stated as:

$\phi(x, y, z, t) \approx \phi(x, y, \bar{z}, t)$ where $\bar{z}$ = average height of the water particles above reference datum. This is equivalent to stating that flow is essentially horizontal so that vertical flow components can be neglected or that the slope of the water table surface is slight ($<5^\circ$).

Now if we assume an incompressible fluid and full saturation then our equation of continuity written in terms of Darcian velocities becomes

$$\frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} + \frac{\partial V_z}{\partial z} = 0 \quad (34)$$

Now since we wish to average in the z direction we must integrate this equation from the base of the aquifer to the free surface or:

$$V_z \bigg|_{z=0}^{z=h} = V_z(h) = -h \left[\frac{\partial V_x}{\partial x} + \frac{\partial V_y}{\partial y} \right] \quad (35)$$

$z = 0 = \text{base of aquifer}$

We may define a potential in terms of head rather than pressure, $\phi_h = P/\rho g + z$. The value of ϕ_h is equal to z at the free surface since $P = 0$ at that point. Using this result along with the first Dupuit assumption and our earlier equation, $z = h(x, y, t)$, we have:

$$h(x, y, t) = \phi_h(x, y, \bar{z}, t) \quad (36)$$

From this result Darcy's law can be rewritten as:

$$V_x = -\bar{K} \frac{\partial h}{\partial x} \quad (37)$$

$$V_y = -\bar{K} \frac{\partial h}{\partial y} \quad (38)$$

where $\bar{K}(x, y)$ = vertically averaged value of hydraulic conductivity at location (x, y)

Substituting equations (37) and (38) into equation (33) we have:

$$n_e \frac{\partial h}{\partial t} - \bar{K} \left[\left(\frac{\partial h}{\partial x} \right)^2 + \left(\frac{\partial h}{\partial y} \right)^2 \right] - V_z(h) = 0 \quad (39)$$

Now replacing $V_z(h)$ with the expression obtained from substituting the results of equations (37) and (38) into equation (35) yields

$$n_e \frac{\partial h}{\partial t} - \bar{K} \left[\left(\frac{\partial h}{\partial x} \right)^2 + \left(\frac{\partial h}{\partial y} \right)^2 \right] - h \frac{\partial}{\partial x} \left[\left(\bar{K} \frac{\partial h}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left(\bar{K} \frac{\partial h}{\partial y} \right) = 0 \quad (40)$$

Rearranging equation (40) yields

$$n_e \frac{\partial h}{\partial t} - \frac{\partial}{\partial x} \left(\bar{K} h \frac{\partial h}{\partial x} \right) - \frac{\partial}{\partial y} \left(\bar{K} h \frac{\partial h}{\partial y} \right) = 0 \quad (41)$$

or in gradient vector notation

$$n_e \frac{\partial h}{\partial t} - \nabla \cdot (\bar{K} h \nabla h) = 0 \quad (42)$$

Equation (41) is termed the Boussinesq equation. To this point for simplicity of development we did not include source terms and have assumed that the aquifer base elevation is the zero reference elevation. To expand Equations (41) or (42) to handle an aquifer with a varying bottom elevation $h_b(x, y)$, and to include source/sink or accretion terms we must do the following:

- Assume that the bottom slope is slight as we did for the free surface slope,
- replace the h in Equations (41) or (42) which was a result of integrating from $z = 0$ to $z = h$ by $h - h_b$ since our integration is now done from $z = h_b$ to $z = h$,

The resulting equation is the Boussinesq equation for unsteady flow:

$$\bar{n}_e \frac{\partial h}{\partial t} = \nabla \cdot \bar{K} (h - h_b) \nabla h + N \quad (43)$$

where

$\bar{n}_e (x,y)$ = vertical average of the effective porosity of the aquifer [dimensionless],

$h (x,y)$ = elevation of the free-surface from some reference elevation [L],

$h_b (x,y)$ = elevation of the aquifer bottom from the reference elevation [L],

$N (x,y)$ = accretion rate [LT^{-1}],

$\bar{K} (x,y)$ = vertically averaged value for hydraulic conductivity at point (x,y) [LT^{-1}]

The Boussinesq formulation as presented above allows one to approximate the elevation of the free surface in a single unconfined aquifer at every (x, y) location. Many times the real system one wishes to simulate is a multiaquifer system where one or more of the aquifers are confined and in addition these confined aquifers may be unconfined in some places. Also there may be transfer between the aquifers. This kind of a multiaquifer system can be handled by a multiaquifer set of Boussinesq equations with potential driven interaquifer transfer or leakage terms. For a two-layered system the equations would be:

$$n_e^1 \frac{\partial h^1}{\partial t} = \frac{\partial}{\partial x} \left[\bar{K}^1 (h^1 - h_b^1) \frac{\partial h^1}{\partial x} \right] + \frac{\partial}{\partial y} \left[\bar{K}^1 (h^1 - h_b^1) \frac{\partial h^1}{\partial y} \right] + N^1 + C_{12}(h^2 - h^1) \quad (44)$$

$$n_e^2 \frac{\partial h^2}{\partial t} = \frac{\partial}{\partial x} \left[\bar{K}^2 (h^2 - h_b^2) \frac{\partial h^2}{\partial x} \right] + \frac{\partial}{\partial y} \left[\bar{K}^2 (h^2 - h_b^2) \frac{\partial h^2}{\partial y} \right] + N^2 + C_{12}(h^1 - h^2) \quad (45)$$

where: superscript refers to aquifer number

$C_{12}(x,y)$ = interaquifer transfer coefficient between aquifer 1 and 2 at location (x,y) . (T^{-1})

In the above formulation the terms $\bar{K}^1(h^1 - h_b^1)$ and $\bar{K}^2(h^2 - h_b^2)$ represent the transmissivity at every (x,y) location. By supplying an interpretation of the position of the confining layer or the top of the aquifer h_t^1, h_t^2 at each x,y location the heads h^1 and h^2 can be compared to h_t^1 and h_t^2 to determine whether the aquifers are confined or unconfined. If they are unconfined then Equations 44 and 45 are used as written. If the aquifers are confined ($h^i > h_t^i$) then the transmissivity is calculated as $\bar{K}^i(h_t^i - h_b^i)$.

Assumptions

The basic assumptions of the Boussinesq flow model in addition to the general model assumptions and those required for describing saturated unconfined flow are:

- Hydraulic conductivity and effective porosity can be represented by the vertical average values,

- the free surface slope and the aquifer bottom slope are both assumed to be slight ($<5^\circ$),
- vertical velocities are assumed to be small and therefore can be neglected,
- coefficient distributions and dependent variables are assumed continuous over the simulation region,
- flow in the capillary fringe is neglected, and
- seepage surfaces cannot be handled and are therefore neglected.

Boundary and Initial Conditions

As with the other models a geometric description of the aquifer extent and aquifer bottom elevation is required. No-flow, flow and known head boundary positions must be specified. The head along the known head boundary must be specified. The recharge/discharge flow rate must be specified along the flow boundaries.

Initial conditions consist of specifying the elevation of the free surface everywhere within the aquifer.

Results Obtainable

Solution of the Boussinesq equation and associated boundary and initial conditions yields an estimate of the vertical average of the potential. In the unconfined case the potential is also the elevation of the free surface. The vertically averaged velocity field is obtainable from the potential, hydraulic conductivity, and porosity distributions.

Limitations

Where significant vertical flow exists, the potential obtained from solving the Boussinesq flow equation will be in error. The existence of a water table (head) or aquifer bottom slope greater than 5 degrees is one indication of significant vertical flow. Significant vertical variation in horizontal flow velocities such as may exist in a layered system may greatly reduce the usefulness of the calculated vertically

averaged velocity field. Such error could have important impact upon transport model predictions. At Hanford, groundwater mounds caused by seepage from disposal sites such as the waste ponds are examples of areas where the Boussinesq approach definitely results in erroneous estimate of the water table height. Continuity of mass is not violated, however, and if the Dupuit-Boussinesq assumptions are valid elsewhere, the Boussinesq flow model should again give good estimates of the water table height at a distance from the discharge site equal to one and a half to two times the saturated thickness.

Where vertical averaging of hydrologic parameters or the other Boussinesq assumptions are not applicable, deviations of the model predictions from true conditions will result. The importance of such error is related to the degree to which reality varies from the assumed condition. At Hanford, the heterogeneous nature of the sediments at least in the unconfined flow system indicates a need to examine the validity of the assumption that the hydrologic parameters can be represented by their vertically-averaged values.

Dimensionality

The nature of the Boussinesq formulation is related to two-dimensional, areal flow. Characteristics of three-dimensional flow may be included by considering several layers with leakage between layers as discussed above.

Applications

A Boussinesq flow model application to the Hanford unconfined aquifer and multiaquifer flow systems can be expected to yield useful potential distributions. This is particularly true for modeling large areas involving hundreds of square kilometers.

CONTAMINANT TRANSPORT

Under this category we include all important factors which may cause differences in the movement of a groundwater fluid and the associated contaminants. Examples of phenomena which are likely to cause such differences are: radioactive decay, ion exchange and other sorption factors, chemical complexing, precipitation, and hydrodynamic dispersion. Earlier we assumed that the transport factors do not affect the fluid flow. In practical terms, this means that the fluid velocity field can be determined over the entire simulation period and the resultant information preserved and input to the transport model at a later time. The prediction of the flow field and contaminant movement are sequential operations under this assumption. A situation where a transport factor influences the flow was mentioned in the beginning of the section on Mathematical Modeling, but the discussion here will be based upon the assumption that flow is independent of transport.

Mathematically the expression of transport as defined here is simply a continuity equation for each chemical species written as:

$$\frac{\partial nC_i}{\partial t} = -(\nabla \cdot C_i \bar{V}) - (\nabla \cdot \bar{J}_i) + R_i; \quad (46)$$

$$i = 1, 2, 3 \dots n \text{ (transport species)}$$

where

C_i = the mass or radioactivity concentration of species i ; $[ML^{-3}]$

t = time; $[T]$

n = porosity [dimensionless]

∇ = the Del operator = $\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$; [dimensionless]

$\bar{V}$ = the mass average Darcian velocity of the fluid; $[LT^{-1}]$

$\bar{J}_i$ = the mass flux of species i relative to $\bar{V}$; $[ML^{-2} T^{-1}]$ and

R_i = the net rate of production or consumption of species i (source/sink term) $[ML^{-3} T^{-1}]$.

The term on the left of Equation 46, is the time rate of change of species i (transient term). The $-(\nabla \cdot C_i \bar{V})$ term is usually referred to as the advective term. This term represents change in concentration of the system resulting from the movement of fluid in which species i is dissolved. The velocity vector of the fluid mixture, $\bar{V}$, is in general a function of time, space, temperature, and the chemical composition of the mixture. If $\bar{V}$ is constant with respect to time, the flow field is said to be steady, if $\bar{V}$ is zero the fluid is stationary.

The $-(\nabla \cdot \bar{j}_i)$ term is often referred to as dispersion and is the macroscopic mixing caused by a combination of the molecular type diffusion, microscopic velocity variations within the pore space flow paths, and small scale variations in advection resulting from the separation of the contaminated fluid into slightly different flow paths. Dispersion causes a given mass of contaminant to spread into a continuously expanding volume of porous medium. Whereas the first two elements of dispersion may be directly related to physical or chemical processes at the microscopic level, the third element is largely a measure of apparent mixing produced by unidentified variations in the porous material which are responsible for changes in the direction and velocity of groundwater flow. The magnitude of the latter component of dispersion is therefore often a function of the scale of porous medium property identification^[10] and becomes more significant as the degree of nonhomogeneity of the medium increases. This type of dispersion has been called macroscopic dispersion^[10]. The combination of velocity variations at the microscopic level and the macroscopic dispersion may be termed mechanical dispersion^[6]. Considerable progress in the field of porous media flow has been made in describing dispersion resulting from molecular diffusion and microscopic velocity variations. This has been accomplished primarily through small column laboratory studies. However, Schwartz states that the ". . . few results that are available from field trials suggest that dispersion effects are considerably more significant than laboratory results would tend to indicate".^[10] The difference between laboratory and field results is caused by macroscopic dispersion. The emphasis in this discussion upon macroscopic dispersion is related to our need to model a

regionally sized, heterogeneous groundwater system and the strong likelihood that macroscopic dispersion is considerably more important than dispersion caused by pore space velocity variation or molecular diffusion.^[10,11] The unidentified variations in the porous material results from the technical and economic difficulties in obtaining sufficient data to completely define the porous medium. The system blocks in a regional model are thus often larger than the true representative elementary volumes (REV). In reality, the mechanical dispersion should be included in the advection term to be rigorously consistent. Since its effect is normally small relative to large scale fluid movement, it is usually associated with molecular diffusion, and included as part of the $-\nabla \cdot \bar{j}_i$ term. The molecular diffusion is composed of ordinary (concentration) diffusion, pressure diffusion, forced (electro-osmotic) diffusion and thermal diffusion. The pressure, forced, and thermal types of diffusion are not normally important in large-scale groundwater problems because of the lack of steep pressure, gravity, electrical or thermal gradients necessary to make these diffusion mechanisms significant in a given problem.

The last term of Equation 46 represents the net production or consumption of species i and is often called the source/sink term. It is the sum of the changes due to reactive or radioactive decay mechanisms and the input or withdrawal of species i associated with the fluid recharge/discharges. Mathematically this can be expressed as

$$R_i = r_i + m_i \quad (47)$$

where

r_i = the net rate of production or consumption of species i by reactive means $[ML^{-3} T^{-1}]$

m_i = the net rate of input/withdrawal of species i such as from a discharge source or pumped well $[ML^{-3} T^{-1}]$.

Some of the reaction mechanisms represented by r_i include ion-exchange, precipitation, complex formation and radioactive decay. The

reactivity of a system may be a function of temperature and any or all of the n mass concentrations in the mixture. This term should in theory consist of a series of rate expressions which represent all known mechanisms by which species i can react in a given system. Species for which r_i is zero are referred to as conservative species since they do not change by reactive means within the groundwater system. Because r_i can in general be a function of all n components of the mixture, it is through this term that the system of n transport equations are coupled. The necessity for obtaining simultaneous solutions of transport and chemistry for all of the constituents present poses a stringent constraint upon the development of a transport model. For most problems of practical interest, the chemical kinetics are simply not known nor are these relationships likely to be obtained in the near future because of the overwhelming experimental problems involved in this type of determination. Often practical solutions of the transport equations can be obtained by assuming that advection-dispersion and reaction occur sequentially within a simulation time step. This simplification can be justified on the basis that groundwater systems in general exist at near chemical equilibria. The reaction rates for most important reactions are extremely rapid with respect to the velocity with which the fluid is moving. Also, the amount of coupling among the equations for different species may be reduced by assuming that trace (contaminant) species do not affect the chemistry of either the significant naturally occurring species or other trace species.

The mass flux of the dispersion term may be expressed as

$$\overline{j}_i = - E^i \nabla C_i \quad (48)$$

where E^i is the coefficient of dispersion of species i and in the general three-dimensional case is a second rank tensor $[L^2 T^{-1}]$.

Equation 46 thus reduces to

$$\frac{\partial n C_i}{\partial t} = - \nabla \cdot C_i \bar{V} + \nabla \cdot (E^i \nabla C_i) + R_i \quad (49)$$

E^i has components defined by

$$E_{xx}^i = D_l^i \cos^2 \psi \cos^2 \theta + D_t^i (\sin^2 \theta + \sin^2 \psi \cos^2 \theta)$$

$$E_{xy}^i = (D_l^i - D_t^i) \sin \theta \cos \theta \cos^2 \psi$$

$$E_{xz}^i = (D_l^i - D_t^i) \sin \psi \cos \psi \cos \theta$$

$$E_{yx}^i = E_{xy}^i$$

$$E_{yy}^i = D_l^i \cos^2 \psi \sin^2 \theta + D_t^i (\cos^2 \theta + \sin^2 \psi \sin^2 \theta)$$

$$E_{yz}^i = (D_l^i - D_t^i) \sin \psi \cos \psi \sin \theta$$

$$E_{zx}^i = E_{xz}^i$$

$$E_{zy}^i = E_{yz}^i$$

$$E_{zz}^i = D_l^i \sin^2 \psi + D_t^i \cos^2 \psi$$

where

ψ, θ are the principal angles between movement caused by convection and the coordinate axes,

$D_l^i = \frac{\alpha_l}{n} |u|$ is the longitudinal dispersion scalar [$L^2 T^{-1}$],

$D_t^i = \frac{\alpha_t}{n} |u|$ is the transverse dispersion scalar [$L^2 T^{-1}$],

$|u|$ is the magnitude of the fluid velocity, [LT^{-1}]

α_l is the longitudinal dispersivity [L], and

α_t is the transverse dispersivity [L].

The dispersivities, α_l and α_t are characteristics of the porous medium alone. Specification of dispersivities is one of the data requirements for a transport model.

Assumptions

In addition to the general model assumptions, the assumptions associated with the transport model above are:

- the total mass density of the solution remains constant.

Other useful assumptions for obtaining practical solutions are:

- chemical equilibrium is established at each time step,
- advection-dispersion and reactive phenomena occur sequentially within each time step of the simulation and,
- many of the trace contaminants do not affect the chemistry of either the significant naturally-occurring species or other trace species.

Boundary and Initial Conditions

The boundary conditions for the velocity fields are supplied to the transport model from an appropriate flow model. If the output of a flow model is potential or pressure, the velocity field must be calculated from potential, porosity, and hydraulic conductivity distributions. In addition to the velocity field boundary conditions the concentration of each transport species of interest must be specified at the flow boundaries.

The initial condition requirements are satisfied when the concentration of each transport species of interest is specified throughout the model region at the beginning of the simulation ($t = 0$).

Results Obtainable

An appropriate transport model will yield the distribution of contaminant mass or radioactivity concentrations throughout the model region as a function of time. In addition, the calculated contaminant fluxes at the discharge boundaries can be provided.

Limitations

When any of the assumptions in this section or under general model assumptions are violated to a significant degree, inaccurate model output will result. The solution of a transport problem over a wide area with a rather detailed grid spacing is often required at Hanford. Under such conditions, a phenomenon known as numerical dispersion can cause errors in the model results for finite-difference or finite-element solution methods. Various Lagrangian solution schemes such as point tracking, particle-in-a-cell or a method developed at Hanford known as discrete-parcel-random-walk have been designed to avoid this problem. Perhaps the most severe limitation in transport modeling arises from the frequent lack of adequate input data. The interaction between various species and the soil matrix can be quite complex and as the number of species of interest increases, the data and parameter requirements can become excessive. As discussed earlier, some simplifications of the chemistry can be useful in obtaining practical solutions.

Dimensionality

Both two- and three-dimensional and, to a limited extent, one-dimensional transport models can be useful. Two-dimensional transport models can be designed to apply to any of the two-dimensional situations mentioned under the preceding flow model discussions. Even in situations where the flow can be assumed to be approximately two-dimensional, however, possible layered flow and/or dispersion in the third dimension may suggest the application of a three-dimensional transport model.

Applications

Some form of a transport model must be used where the location, concentration, and/or discharge fluxes of contaminants are required and where differences exist between the movement of the groundwater and the

associated contamination. If it can be shown that the shortest ground-water travel time from a waste disposal site to a biospheric uptake point is such that radioactive decay will reduce all contaminant activity to a harmless level, application of a transport model may not be necessary.

MATHEMATICAL SOLUTION METHODS FOR FLOW AND TRANSPORT PROBLEMS

A wide variety of mathematical solution methods are available for application to groundwater flow and transport problems. Many such methods are analytical or semianalytical techniques applicable to quite simplified equations and associated boundary and initial conditions. Although such techniques allow one to adequately and rapidly solve many simple problems, the solution of the more realistic equations presented herein over wide areas with complex boundary and initial conditions such as often exist at Hanford are usually beyond analytical or semianalytical methods. Transforming the mathematical formulations of the models as presented herein into practical predictive tools usually requires the application of numerical solution methods in the form of sophisticated computer codes. The development of such codes is normally based upon the subdivision of one or more of the equation spatial variables into a series of control spaces (control volumes for three-dimensional cases, control areas for two-dimensional, etc.) The appropriate model equations are applied to each of the discrete units and coupled to the appropriate equations of its nearest spatial neighbors. Matrix algebra and iterative techniques are usually employed to solve the set of equations (at least one equation for each control space) with appropriately specified boundary and initial conditions. Measured values or estimates for the equation parameters such as hydraulic conductivity, porosity, diffusivity, etc. are specified at each control space and the calculated values of the equation dependent variables (potential, pressure, contaminant concentration, etc.) are output for each control space. Both the model input and output values are semicontinuous in that they are usually only specified at each control space. Smaller spacing results in a more continuous and precise solution but requires more input data and more computer resources.

The numerical approach to problems with time-varying conditions (transient problems) requires a subdivision of time into discrete intervals as well as the spatial discretization. The entire set of spatial equations are solved at each time step although the results of a nearby (usually the previous) time step influence the calculation. In this manner the model output at each control space may change with time. As with spatial discretization, a finer time step results in a more precise solution in time at a higher cost in computer resources. Additional data requirements for a transient problem involve more frequent measurements or estimates of the time-varying conditions such as the boundary conditions, discharges, and recharges.

SELECTED COMPUTER CODES POTENTIALLY APPLICABLE TO HANFORD

Considerable development during recent years has led to improved analysis methods and computer models potentially useful in the management of the Hanford groundwater system. These developments are dispersed in governmental agencies, research organizations, water resource consulting firms, petroleum consulting firms, state agencies and universities in the United States and throughout the world. Although widely dispersed, offsite analysis tools applicable to Hanford needs offer a major potential benefit and economy in upgrading Hanford groundwater modeling capability. Accordingly, a model inventory was initiated to identify and, insofar as possible, evaluate those computer codes most applicable to the Hanford situation as set forth earlier in this report.

A detailed literature search and replies from mailed inquiries are the basis of the additional information assembled on groundwater modeling and analysis methods. The literature search of some 1400 references yielded 522 papers, abstracts or summaries closely associated with groundwater modeling. From 567 mailed inquiries to complement the literature search, 139 responses were received with specific information on computer codes.

From the collected information 36 groundwater computer codes have been selected as being of possible application to Hanford needs. If more than one code of similar type was located, all were included if they were potentially useful in filling Hanford needs. However, some codes were purposely omitted since they were not particularly needed at Hanford. As an example, no salt water intrusion code was included in those selected.

The selected models are conveniently considered and discussed in the grouping used earlier in the report; namely, those models used in:

- (1) fluid flow determinations, and
- (2) contaminant transport analysis.

The computer codes useful in these areas are discussed in detail in the Appendix-Model Inventory.

FLUID FLOW DETERMINATIONS

The flow determinations involve evaluating changes in groundwater movement. These changes may result from proposed management practices or simply from natural trends in the subsurface flow regime. In any case, the new flow system conditions are obtained through setting up and solving appropriate well-posed boundary value problems. Such boundary value problems are the basis of flow determinations using a code.

In Figure 12 which resembles Figure 7, the fluid flow systems are divided into 3 classes of saturated flow, partially saturated flow, and multiphase flow conditions. Under each of these flow-system types are listed the computer codes considered potentially helpful for Hanford use. In many cases, the specific name appearing in Figure 12 for each code was originated by the present authors for the purposes of brevity and to allow easy reference to the Appendix.

FLUID FLOW

SATURATED

<u>Confined Aquifer</u>	<u>Unconfined Aquifer (Free Surface Representation)</u>	<u>Boussinesq Approximation</u>	<u>Partially Saturated (Static Air, Dynamic Water Phase)</u>	<u>Multiphase (Dynamic Gas and Water Flow)</u>
INTERA-HCTM	INTERA-HCTM	HANFORD-VTT	COLORADO FD	INTERCOMP-GWM
DAVIS FE	WALES, Eng.	COOLEY	SEGOL FE	KANSAS-GREEN
TRUMP	USGS (3D)	ISOQUAD2	OAK RIDGE FE	ARCO-IMPES (5C)
FLUMP	FRESURF 1 & 2	SPASM, Ill.	NEUMAN FE	
SOPH	MASS, Isr.	SAMMIR-Fr.	USFLW, Isr.	
MICHIGAN		MASS, Isr.	INFIL, Fr.	
		WEBER		
		MICHIGAN		
		HIGH PLAINS		

FIGURE 12

OFFSITE AND ONSITE FLOW MODELS OF POTENTIAL USE AT HANFORD

Confined Aquifer Saturated Flow

The saturated, confined flow system modeling capability is applicable in shallower, confined and deeper basalt interbed situations. The simplifying feature in such systems lies in not having to determine both the free surface shape (water table) and the flow field potential distribution together. In confined systems the overlying stratum provides the upper flow boundary so only the potential distribution beneath the confining layer need be determined by the model.

There are six potentially useful models for confined flow situations. The first three of the six models listed in Figure 12 are capable of considering three-dimensional flow systems, whereas the last three are limited to considering two-dimensional situations. Of those considering two dimensions only the FLUMP program can consider flow in a vertical plane with gravity effects. The other two models are restricted to flow in essentially the two-dimensional horizontal plane.

Unconfined Aquifer--Free Surface Representation Saturated Flow

The unconfined saturated flow condition where the free surface (water table) must be determined as part of the model solution is among the most common situations encountered at Hanford. The computer codes in this category are listed in the second column of Figure 12. The method of solving for the free boundary condition represents one of the important differences among these codes. Several of the listed codes solve the free boundary condition in some fashion whereas others approach the free boundary problem by adjusting the effective thickness of the upper block to the saturation thickness of that block. It is likely that most or all of these codes are applicable to confined flow by suppressing the feature which deals with the free surface. Conversely, it is likely that some of the confined aquifer codes listed in the first column of Figure 12 can be adapted to include free surface solution methods.

Unconfined Aquifer--Boussinesq Saturated Flow

The third column of Figure 12 contains a list of the Boussinesq Type computer codes which have applicability to Hanford. Several of the offsite codes utilize the finite element method which offers some advantages over the finite difference method used by the onsite code (Hanford VTT). Otherwise, the offsite Boussinesq flow codes do not appear to have significant advantages over the Hanford code.

Partially Saturated Flow

The partially saturated flow computer codes which were felt to be of potential benefit at Hanford are listed in the fourth column of Figure 12. In general, the only codes considered in this category are those which follow the formulation presented earlier under the mathematical model section wherein the equation was developed such that it could be reduced to a saturated flow equation. The point was made that both the partially saturated flow and multiphase flow models as presented would be applicable to a system involving zones of partial saturation and full saturation. Other codes are available which apply strictly to the partially saturated zone using a moisture content formulation. None of the moisture content partially saturated codes have been included because of their limited applicability.

Although an onsite code was prepared in this category^[12], the effort was directed towards obtaining insight into partially saturated phenomena and the model was never developed into an operational management tool.

None of the codes identified under this category seems capable of being applied to the full range and scale of problems expected in the Hanford environment.

Multiphase Flow

The applicable multiphase codes identified to date are listed in the final column of Figure 12. Several of these codes were developed

for the petroleum industry. Other proprietary multiphase flow models undoubtedly exist within the various petroleum companies. The successful application of multiphase models by the petroleum industry to a variety of rather complex problems is an indication of a substantial degree of development and reliability of multiphase type models.

CONTAMINANT TRANSPORT ANALYSIS

The computer codes which may be applicable to contaminant transport at Hanford are listed in Figure 13. Several of these are codes wherein the flow and transport equations are solved together in the same program, hence the repetition of some of the same codes from Figure 12. Many of these codes are limited to conservative species transport. Many also employ an Eulerian grid system (fixed-in-space) which although quite useful in many applications is likely to suffer from numerical dispersion when applied to the Hanford system. The only code identified to date which is applicable to a large multicomponent, nonconservative system while at the same time employing a Lagrangian grid system is the Hanford MMT-DPRW^[13]. The MMT-DPRW code utilizes a method of assigning a value for the contaminant mass to each parcel which the developers claim eliminates mass balance problems associated with some Lagrangian transport methods. In addition, this model is designed to utilize a flow velocity field from a variety of flow models. Several of the other codes listed on Figure 13 contain attractive methods and routines which benefit transport modeling at Hanford.

NUMERICAL METHODS OF OBTAINING IMPROVED DATA DISTRIBUTIONS

One of the most difficult and expensive tasks involved in groundwater modeling is the collection of adequate field data. For this reason it can be quite useful to cause a model to provide estimates of aquifer characteristics by supplying it with measurements or estimates of the parameter which is normally the model output. For example, the hydraulic conductivity (K) distribution obtained from pumping tests may

CONTAMINANT TRANSPORT

CONSERVATIVE CONSTITUENTS		REACTIVE CONSTITUENTS	
Advective Changes Only	Advective and Dispersive Induced Charges	ADVECTIVE AND DISPERSIVE CHANGES WITH:	
		Equilibrium Reactions	Kinetic Reactions
HANFORD, PCP FLOP 1 & 2 FRONT	INTERA-HCTM	MMT-DPRW	MMT-DPRW
	SEGOL	SCHWARTZ	
	USGS, MC	REFQS	REFQS
	ISOQUAD	OAK RIDGE, FET	
	USFLW, Isr.	USFLW, Isr.	

FIGURE 13

OFFSITE AND ONSITE TRANSPORT MODELS OF POTENTIAL USE AT HANFORD

be improved by providing a potential distribution obtained from well measurements to a saturated flow model which has been reformulated to solve for the hydraulic conductivity rather than for the potential. Once a good distribution for K has been determined, the model can be applied in the normal sense to obtain a prediction for the potential distribution with different boundary recharge, or discharge conditions. Since under Darcian flow assumptions the hydraulic conductivity is a function only of the solid medium and liquid characteristics, changing flows would not be expected to cause variations in the K distribution. Another approach along these lines involves the use of the actual computer code to historically match known data (such as potential) by varying one or more parameters for which measured data are limited or nonexistent. Once the historical data are matched as well as possible it is assumed that the parameter estimates used are accurate. Such a history matching approach can be performed by trial and error or by the assistance of auxiliary codes which automatically seek the optimum parameter distribution.

A number of codes exist which either directly solve for aquifer parameters or which assist in history matching.^[14,15,16,17,18] We term such codes parameter identification codes.

Parameter identification codes are useful at Hanford where approximately 400 wells are routinely monitored for either water level, contaminant concentration or both, but where the number of useful aquifer parameter (particularly transport parameter) measurements are limited.

AUXILIARY COMPUTER CODES

Auxiliary capability falls into one or more of the following categories:

- 1) routines which accept more or less raw data and prepare them into a form acceptable to a major code,

- 2) routines which display collected data or the results of a simulation in an understandable and convenient form, and
- 3) codes which solve quite simplified problems much more rapidly and economically than one of the sophisticated codes.

In the past, emphasis has been placed upon man-computer interaction for rapid analysis and decision making. For example, a set of routines which provide immediate display of model predicted groundwater potentials and/or contaminant distributions in the form of contours upon a Hanford map has proven to be a great deal more rapid and convenient than the typical situation where pages of numbers must be analyzed and then hand plotted. Another example of auxiliary codes which have demonstrated their value in the Hanford groundwater modeling program are a series of auxiliary routines which can quickly plot prepared input data to assist in identifying data errors prior to expensive model simulations.

In general, the use of auxiliary routines or models as described above can be a valuable asset to the Hanford groundwater modeling program.

CONCLUSIONS AND RECOMMENDATIONS

At Hanford we have a set of operational flow ^[5] and transport ^[13] codes which allow us to model the unconfined aquifer in two-dimensional, horizontal space. A two-dimensional parameter identification code for calculating a hydraulic conductivity distribution throughout the Hanford Reservation is also available. ^[18] These models have been tested using synthetic cases and verified as far as possible using actual Hanford field data. Additional modeling capability needed at Hanford includes the following:

- (1) a multiaquifer model which would permit the treatment of the groundwater flow system as a set of interconnected aquifers,
- (2) models which would allow a true three-dimensional simulation of both the flow and contaminant transport phenomena within certain sections of the Hanford Reservation,
- (3) capability to accurately predict flow and transport within the partially saturated zone, and
- (4) increased capability to determine distributions of such aquifer parameters as hydraulic conductivity, effective porosity, and chemical sorption coefficients from a minimum number of field measurements.

The onsite two-dimensional flow code (Hanford VTT) has multi-aquifer capability and can be used in the initial stages of extending the Hanford modeling and data collection effort into the confined (regional) aquifer system. Later as the definition of the various Hanford aquifer systems is refined, adaptation of offsite multiaquifer models and/or some limited additional development may become necessary.

In order to satisfy in part the additional modeling needs as outlined above, the most promising modeling capability available offsite will be adapted to the Hanford groundwater modeling environment. The

entire suite of models will be used to assist in defining the flow and contaminant transport behavior underlying the Hanford nuclear waste facilities and to assist waste management decision making. The modeling program will be interfaced with the Hanford subsurface characterization programs in order to obtain best results. If important modeling needs remain unsatisfied subsequent to adaptation and testing of available offsite models, plans will be formulated to develop additional modeling capability.

A limited amount of refining and improvement of the present onsite models will be performed as needed and as additional data become available. Development and implementation of additional auxiliary codes for the purposes outlined under AUXILIARY COMPUTER CODES will be conducted as needed to assure maximum efficiency in data analysis and groundwater modeling.

REFERENCES

1. R. A. Deju, R. E. Gephart, "Hydrologic Management at the Hanford Nuclear Waste Facility," ARH-SA-235, Atlantic Richfield Hanford Company, Richland, Washington, 1975.
2. V. T. Chow, "Laboratory Study of Watershed Hydrology," Proc. Int. Hydrol. Symp. 1, Fort Collins, Colorado, 1967, pp. 194-202.
3. A. Hunter Blair, "A Groundwater Analogue Investigation of a multi-well pumping scheme at Otterbourne (Southampton Corporation Waterworks)," Water Res. Assoc., Medmenham, Tech. Pap. 56, 1966, pp. 71.
4. C. C. Kisiel, "Time Series Analysis of Hydrologic Data," Advances in Hydroscience, Academic Press, New York and London, 1969, pp. 119.
5. K. L. Kipp, A. E. Reisenauer, C. R. Cole, and C. A. Bryan, "Variable Thickness Transient Groundwater Flow Model Theory and Numerical Implementation," BNWL-1703, Battelle Pacific Northwest Laboratories, Richland, Washington, 1972 (Updated 1976).
6. J. Bear, "Dynamics of Fluids in Porous Media," American Elsevier, 1972.
7. J. H. Dane, "Effect of Hysteresis on the Prediction of Infiltration, Redistribution and Drainage of Water in Large Soil Columns," M.S. Thesis, Department of Agronomy, New Mexico State University, Las Cruces, New Mexico, 1972.
8. P. C. Trescott, "Documentation of Finite-Difference Model for Simulation of Three-Dimensional Groundwater Flow," U. S. Geological Survey Open File Report 75-438, September 1975.
9. P. W. France, "Finite Element Analysis of Three-Dimensional Groundwater Flow problems", Journal of Hydrology, vol. 21, no. 4, 1974, pp. 381-398.

10. F. W. Schwartz, "Macroscopic Dispersion in Porous Media: The Controlling Factors," University of Alberta, Edmonton, Alberta, Canada, submitted to Water Resources Research, June 1976.
11. R. A. Greenkorn and D. P. Kessler, "Dispersion in Heterogeneous Non-Uniform Anisotropic Porous Media," Ind. and Eng. Chem, vol. 61, no. 9, p. 14-32, 1969.
12. A. E. Reisenauer, D. B. Cearlock, and C. A. Bryan, "Partially-Saturated Transient Groundwater Flow Model Theory and Numerical Implementation," BNWL-1713, Battelle Pacific Northwest Laboratories, 1973.
13. S. W. Ahlstrom and H. P. Foote, "Multicomponent Mass Transport-Discrete Parcel Random Walk Model Theory and Numerical Implementation," BNWL-2127, Battelle Pacific Northwest Laboratories, to be published December, 1976.
14. Y. Emsellem and G. DeMarsily, "An Automatic Solution for the Inverse Problem," Water Resources Research, vol. 7, no. 5, October, 1971.
15. W. W-G. Yeh, "Aquifer Parameter Identification," Jour. Hydraulics Div., ASCE, September, 1975.
16. Y. Y. Haimes, "Hierarchical Management of Ground and Surface Water System Via Multicell Approach," Case Western Reserve University, Cleveland, Ohio, July 1975. Available from National Technical Information Service, Springfield, Va., as PB247-100.
17. D. McLaughlin, "Investigation of Alternative Procedures for Estimating Groundwater Parameters," Water Resources Engineers, Walnut Creek, California, January, 1975. Available from National Technical Information Service, as PB239-952.
18. D. B. Cearlock, K. L. Kipp, and D. R. Friedrichs, "The Transmissivity Iterative Calculation Routine - Theory and Numerical Implementation," BNWL-1706, Battelle Pacific Northwest Laboratories, 1972, (revised 1976).

APPENDIX

MODEL INVENTORY

The 36 computer codes selected as being potentially applicable to Hanford needs as discussed in the text are treated individually in this Appendix.

The individual code discussions are grouped according to the categories shown in Figures 12 and 13 of the text.

SATURATED FLOWConfined Flow

INTERA-HCTM

Of the three-dimensional models, the commercial proprietary INTERA-HCT Model has likely been used upon the largest variety of saturated flow problems. This program, which is more generally known as the Intercomp/ Inter-a-Hydrologic Contaminant Transport Model, has its origin in earlier petroleum reservoir engineering analysis.^[1,2] From this background comes the formulation that includes the effects of the fluid and material compressibility. Such effects are more important with the larger pressures and pressure differences usually present in petroleum reservoirs. The compressibility of water and the porous material are of less importance in groundwater aquifers due to the smaller pressures involved. Since minimal additional input is required for compressibility effects, there is little inconvenience in considering the slight compressibilities involved. Also, from the petroleum background comes a flavor of emphasis on wells and several convenient ways of including them in a saturated model.

The model utilizes finite differences with emphasis on a block type formulation, as contrasted to a nodal emphasis or representation. Accordingly, the representation is more in the setting and has the

advantages of the "Integrated Finite Difference Method" (IFDM) that are referenced later in this section in connection with the TRUMP model. The actual solution of the once integrated difference equations is accomplished either by standard line successive over-relaxation (LSOR) techniques for larger problems, or through using a special equation ordering scheme followed by direct Gaussian elimination.

The rectangular blocks used in the model may vary in size as desired by the user within two overall guidelines. First, the blocks must include the entire flow system volume of interest, and second, once a particular block width, length, or depth is used, it is generally advisable to continue that block dimension if that direction is an expected major direction of flow. The flow characteristics or properties of the material may be assigned differently in every block in the flow system. The block potentials may also be held to a specified potential history, and wells can be positioned at essentially any desired location within or through blocks. For example, wells need not be located at the block center and withdrawals can be from perforated well bore sections at different depths, i.e., they may lie in one or more different vertical blocks. The well potential can be set by the user, or the well bore or flow rate may be specified directly.

All of these features make the model a very flexible predictive tool. It also has the advantage of having been applied to a variety of practical problems which has enhanced the flexibility and applicability of the model. The flow model is directly coupled to a transport model for handling conservative constituents.

DAVIS FE

The DAVIS FE model is a three-dimensional model developed by S. K. Gupta while with the Water Science and Engineering Section, University of California at Davis.^[3] The model considers saturated confined flow in three dimensions with both the fluid and porous material considered compressible. The time dependence arising from

compressibilities is considered through a backward difference and the spatial discretization is through finite elements.

Three-dimensional isoparametric elements are used that can be deformed in any of the three coordinate directions. The spatial basis functions for the isoparametric shapes along any element edge may be either linear, quadratic, or cubic in functional form. Such functional forms are incorporated by inserting additional node points along the element edge, i.e., the two end points are used for the linear form, adding a node at the center provides the quadratic variation, and the cubic is obtained through adding internal nodes at the one-third points along the element side. This procedure allows flexibility, particularly in satisfying irregular boundary conditions, yet maintains the advantages of using the simpler Chapue basis functions for the potential or head representation.

The model was designed for use on a small to intermediate size computer, so the potential determination aspects utilize four of the five subprograms. The first subprogram, FE/PREP, is a preparation routine for setting up the problem, getting all the soils, boundary, and initial condition input and organized for use by the FE/HEAD subprogram. This second subprogram actually sets up the equations requiring solution and very efficiently organizes the resulting matrices through optimal ordering for efficient solution in the subprogram FE/GAUSIN. The small subprogram FE/FLUX complements the HEAD program by providing flux results as required most extensively in transient problems. The last subprogram solves the transport equations using finite elements, but is of limited utility at Hanford.

The only field application of the model since it was developed during the last two years has been the Sutter Basin in California. It is at the present time being applied to Long Island, New York.

TRUMP

The TRUMP model is actually a computer program for transient and steady state temperature distributions in multidimensional systems that

has been used in subsurface flow and involves Integrated Finite Difference Methods (IFDM)^[4]. The (IFDM) methods have been widely used effectively for some time, apparently developing during the early 1960's from the engineer's feel for the physical system, and have only more recently gained the respectability of formal mathematical derivation. Such methods are similar to the Galerkin finite element approach and the best features of both may be incorporated into future improved models.

FLUMP

The FLUMP model evolved from the TRUMP model already discussed, though it has been further modified considerably by S. P. Neuman.^[5,6] It is considerably easier to use on groundwater flow problems than is TRUMP, though it is restricted to two-dimensional flow in either vertical or horizontal planes. FLUMP uses a finite element numerical scheme which has been shown^[4] to represent only a small change from the original approach used in TRUMP.

SOPH

The SOPH model, i.e., Simulation Of Piezometric Head model, is for use with two-dimensional lateral flow in a completely confined situation.^[7] Only confined cases are treated with this particular model, which apparently has been used rather widely by the Ontario (Canada) Department of the Environment during the past two years. The computer model involves use of finite differences with the algebraic equations solved using an alternating direction implicit procedure (ADIP).

MICHIGAN

The MICHIGAN model is a two-dimensional finite element model for flow in the x, y plane with no direct gravity effects. The model was developed at Michigan State University by D. C. Wingert of the Civil Engineering Department.^[8] The model has been used only on the Michigan State University Water Quality Management Facility. The model appears particularly well suited to handling variable pumping and artificial recharge or injection well inputs.

Unconfined or Free Surface Flow

INTERA-HCTM

The INTERA-HCTM three-dimensional model, which was described in the previous section, has been recently modified to approximately handle free surface problems. The modifications allow the uppermost block to automatically adjust so only the required saturated thickness of the top block is utilized. This approximate treatment is highly dependent upon the block size, both vertically and horizontally. If large blocks are involved to represent a big flow system, then the water table approximation is poorer. In every other respect, the HCT Model is the same as described in the previous section on confined saturated models.

WALES-Eng.

The WALES-Eng. model was developed by P. W. France of the Civil Engineering Department at the University of Wales Institute of Science and Technology.^[9] It is a three-dimensional finite element formulation for saturated flow of an incompressible fluid in nondeformable porous material. This yields the elliptic type partial differential equation valid for both steady and transient flow problems. In the transient flow systems, the time dependence enters through time varying boundary conditions, one of which may be the free surface. Accordingly, the transient free boundary is treated as a discrete number of steady flow problems to affect the time varying free surface. A carefully devised elemental formulation approach is used to calculate the normal velocity of the free surface, and to adjust the free surface to the new location during the time increment. The revised locations of the finite element nodes lying on the new free surface are next calculated using a Newton-Raphson iterative method. With the new locations of the boundary finite element nodes known, the standard three-dimensional Galerkin finite element solution method is used to obtain the groundwater potential distribution throughout the region. Cubic isoparametric elements are used to permit accurate representation of irregular and curved boundaries.

This approach is the most direct analytical combined approach to the solution of free boundary problems in three dimensions. The approach was validated by the developer, utilizing analytical radial symmetrical solutions before adapting the method for general use.

USGS (3D)

The USGS (3D) model is a three-dimensional finite difference program that has evolved under the guidance of Peter Trescott from the earlier U. S. Geological Survey programs based upon the two-dimensional Boussinesq Approximations.^[10] From this earlier background, there remains a mixed use of the transmissivity concepts in the x and y coordinates directions and hydraulic conductivity times a thickness parameter in the z or vertical coordinate direction. Also, the source and storage terms must be specially considered by the user, since they assume a pseudo two-dimensional connotation. The program uses the strongly implicit procedure (SIP) described by Stone^[11] for two-dimensional problems and extended by Weinstein, Stone, and Kwan^[12] to three-dimensional systems. Likely, this model would be most useful when representing thick confining beds where storage changes are very significant.

FRESURF 1 & 2

The model was already described in the preceeding section. The specifics of the free boundary are described in Neuman^[5] and are incorporated into the finite element solution scheme used in this two-dimensional model. The free boundary is handled by the finite element network, expanding or contracting to accommodate the movement of the free surface with time. The total derivative of the potential, with respect to time, is combined with the specific free boundary conditions which are substituted into the generalized variational principle for the saturated flow problem to give the expression for the free surface. This expression is a set of nonlinear ordinary differential equations. A Crank-Nicholson time centered scheme is used to solve the non-steady

flow with the free surface. The regular finite element approach, based upon the variational principle, provides the potential distribution below the free surface.

The above features for handling the free surface and potential distribution are used in the model to solve both two-dimensional and axisymmetric flow problems. The program also solves for the seepage face, if one occurs, through a two step iterative procedure. It would appear that considerable additional development would be required to extend the procedure to a three-dimensional situation. Since it is two-dimensional, the predictions are restricted to only vertical sections when the free surface feature is utilized.

MASS-Isr.

The MASS-Isr. model which is an acronym for Multi-Aaquifer Simulation System (Israel) is one of a group of models developed under J. Schwarz, Head of the Research and Development Section, Hydrology Division of TAHAL, in Israel.

Boussinesq Approximation

HANFORD-VTT

The HANFORD-VTT model, more generally known as the Hanford Variable Thickness Transient flow model, has been used on a variety of practical flow problems. It has been developed and improved over a number of years by the Battelle Pacific Northwest Laboratory staff in Richland with major development funding from the Atlantic Richfield Hanford Company.^[13] The model originated from a standard finite difference Boussinesq formulation, but has been enhanced as various problems have been solved so that today it is an elaborate and extensive evaluation tool. It has multi-aquifer capability with variable thickness features for the unconfined strata and can solve both transient and steady state problems. More detailed solution at a finer difference grid spacing is possible by a sequential solution process wherein the results of a large region simulation are used as boundary conditions for a smaller region.

The model is part of a flexible interactive subsurface evaluation capability. Part of this interactive flexibility centers upon extensive input assistance and checking features to assure the problem is free of input inconsistencies. The extensive output capabilities are most useful in effectively demonstrating the solution process for complex problems.

COOLEY

The COOLEY model was developed by Richard L. Cooley, originally at the Center for Water Resources Research in the Desert Research Institute at the University of Nevada, and more recently with the U. S. Geological Survey in Denver.^[14] The model is particularly well documented in regards to the theoretical formulation, the reduction to finite elements, the matrix solution methods, program listings, and even example test cases. A direct finite element approach is used for the reduction to numerical form, with four matrix solution options being incorporated into three different computer programs. The Line Successive Over-Relaxation (LSOR) and Corrected Line Successive Over-Relaxation (LSORC) Techniques are used together in one program. The two methods are together in the same program since the correction feature in the LSORC method cannot be used with certain boundary conditions. The other two programs use the Iterative Alternating Direction Implicit Procedure (ADIPIIT) and the Strongly Implicit Procedure (SIP), respectively, for matrix solution.

ISOQUAD2

This is the Galerkin Finite Element Model developed by G. F. Pinder of Princeton University and the U.S. Geological Survey and E. O. Frind of the University of Waterloo, Waterloo, Ontario, Canada. The approach used by Pinder and Frind is well described and has been rather broadly applied by several investigators. In the paper describing this model^[15] a comparison is made between the Galerkin finite element method using mixed isoparametric elements and a comparable finite difference approach. The primary advantage of the Galerkin approach lies in the

flexibility provided by the use of irregular subspaces and an integration scheme permitting the use of higher order deformed elements. These advantages must be weighed against the very efficient equation solving schemes applicable to the finite difference equations. An updated version of the Pinder model describes transient, two-dimensional groundwater flow including the effects of vertical transient leakage from a confining layer.^[16] A mass balance calculation was recently added by P. C. Trescott of the U. S. Geological Survey, Reston, Virginia.^[16]

SPASM, Ill.

The SPASM, Ill. model was developed by the Illinois State Water Survey under the guidance of T. A. Prickett.^[17] The distinguishing feature of this model, which has been in use for some time, is the flexibility provided through the set of compatible subroutines that may be combined very easily to provide the desired solution capability.

SAMMIR, Fr.

The SAMMIR, Fr. is a French model developed by a group at the Center of Geological Information of the National Department of Mines in Paris.^[18] The model simulates multilayered aquifers with a set of nesting square meshes. Emphasis is upon considering a number of distinct aquifers of large lateral extent having vertical connections with one another by leakage. The model has apparently been used upon a number of field problems in Europe.

MASS, Isr.

The MASS, Isr. model was discussed previously in the section on saturated unconfined flow.

WEBER

The WEBER model was developed originally in the early 1960's by E. M. Weber of the Los Angeles District of the California State Department of Water Resources.^[19] With continuing use, the model has evolved

from the original linear formulation to the nonlinear variable thickness model of today. The model has been rather widely used on many problems under the jurisdiction of the California Department of Water Resources.

MICHIGAN

The MICHIGAN model, which was described under the previous topic of confined saturated flow, also utilizes the lateral flow part of the Boussinesq Assumptions to estimate the free surface shape under unconfined situations.

HIGH PLAINS

The HIGH PLAINS model had its conceptual origin from the first WEBER model with actual development and subsequent enhancement by the Civil Engineering Department of Texas Technical University in Lubbock, Texas.^[20,21] The model was specifically designed and has been applied primarily to the part of the Ogallala aquifer controlled by the High Plains Underground Water Management District No. 1 in Lubbock, Texas. The model uses a finite difference approach with straight iterative solution of the difference equations.

PARTIALLY SATURATED FLOW

COLORADO, FD

The COLORADO, FD model was developed at Colorado State University originally by William F. Brutsaert with guidance from E. A. Bretenbach.^[22,23] The model has evolved to handle three-dimensional problems, though originally restricted to two-dimensional systems. It is a finite difference model which uses a Newton iteration method in preference to the less stable forms examined by Brutsaert^[24] in some detail. The use of upstream weighting of the capillary conductivity is utilized with the Newton iteration to provide a stable solution method. The model was applied in a three-dimensional simulation of the partially saturated zone of a 40 mile reach of the Arkansas River of southeastern Colorado.^[25] The saturated zone was treated by applying a two-dimensional Boussinesq type model. The model as adapted for use in this

stream-aquifer system model provided water table elevations that agreed reasonably well with observed data. This combination of models from the information now available, has been applied to the largest region and to the most complicated set of field conditions of any of the partially saturated flow models located.

SEGOL, FE

The SEGOL, FE model was formulated and written by Genevieve Segol, who earlier was at Princeton associated with Pinder and more recently at Waterloo University.^[26] The model solves for three-dimensional combined partially saturated and saturated flow. Since solution for both saturated and partially saturated flow is possible, the free surface is very nicely handled. At the same time, a more realistic representation of flow from ponds or lakes is provided by the model, rather than requiring the assumptions involved when only saturated models are used. The SEGOL model utilizes finite elements for the numerical reduction with isoparametric elements. It is an operational model and has been tested, but has not yet been extensively used with field problems. A severe test case involving imbibition led the author to indicate that a spatial discretization of a few centimeters may be necessary for such problems.

OAK RIDGE, FE

The OAK RIDGE, FE model was developed under National Science Foundation support at the Oak Ridge National Laboratory by M. Reeves and J. O. Duguid. The development effort and model are particularly well documented.^[27] The model handles combined partially saturated and saturated flow in two-dimensional transient situations. The model development effort appears to have grown out of the developers experience using the partially saturated flow model of R. A. Freeze of IBM.^[28] Like most of the Freeze applications, the OAK RIDGE, FE model has been applied to either drainage cases or those with rather moist initial conditions. Such cases are much less likely to experience instabilities in numerical solution.

The program is a finite element Galerkin model with isoparametric elements for the spatial integration and performs the time integration using a modified Crank-Nicholson type method with a moving location between 0 and Δt for calculating the time derivatives. In fact, the variable location along Δt can be selected to get greater stability if needed. The nonlinear capillary conductivity and saturation dependence upon the pressure head is handled by repeated cyclic solution. The dependent properties are updated compatible with the last calculated pressure heads followed by recycling through the efficient matrix solution steps to get new pressure heads with which to revise capillary conductivities and saturation again. Such a cyclic process could get into stability difficulties on imbibition problems with very low initial moisture contents. Unfortunately, it is this more difficult class of problems upon which the model apparently has not been tried.

NEUMAN, FE

The NEUMAN, FE model developed by S. P. Neuman can handle saturated and partially saturated flow in a vertical plane, horizontal plane, or with radial symmetry.^[29,30] It is a finite element Galerkin method of numerical reduction. The seepage surfaces are handled directly by this model, which could not be done in any of the previous models described in this section. Specifically, the position of the exit points on the seepage faces are adjusted automatically during each time step. It appears from presently available information that application has involved mostly calculation of flow through earth dam type problems with sloping cores and drain blankets, rather than extensive field type problems.

USFLW, Isr.

The USFLW, Isr. model is one of the group of models developed and being used under J. Schwarz, Head of the Research and Development Section, Hydrology Division of TAHAL, in Israel.

INFIL, Fr.

The INFIL, Fr. model was developed by George Vachaud of the Institute de Mecanique, Grenoble, Cedex/France. It is a combined saturated and partially saturated flow model with special infiltration analysis capabilities.

MULTIPHASE FLOW

INTERCOMP-GWM

The INTERCOMP-GWM model is more generally known as the Intercomp Gas Water Model and was prepared under the direction of K. H. Coats of INTERCOMP Resource Development and Engineering, Inc., Houston, Texas. It is a three-dimensional model describing the simultaneous immiscible flow of water and air. Any combination of reduced conditions can be treated, i.e., it may consider completely saturated flow in parts of the flow system, or conversely, if essentially no water is present, then the gas flow is evaluated.

The Gas-Water Model uses finite differences for numerical reduction of the partial differential equations and the resulting algebraic equations are solved, using either a line successive over-relaxation (LSOR) or a special ordering scheme followed by direct Gaussian elimination. Though either solution may be used the special ordering with Gaussian elimination is preferred for most systems. In very large systems, the LSOR method may be required.

There are two versions of the model, one of which is likely to be of greatest usefulness in fulfilling the regional Hanford needs outlined in the body of this report. This is the IMPES version which is an Implicit in Pressures and Explicit in Saturation scheme which saves from 1/2 to 1/3 in computer running time to provide a solution. The second, more costly version involves completely simultaneous solution, a capacity likely not generally required for the regional Hanford use. The INTERCOMP oil-gas-water model, from which this gas-water model evolved as a special case, has been used extensively in evaluation of a variety of

petroleum reservoirs. The present gas-water model is also being applied to an ever greater number of subsurface gas-water problems.

KANSAS-GREEN

The KANSAS-GREEN model was developed at the University of Kansas as part of the Water Resources Research Institute Program.^[31,32] It is one of the very few water resource oriented models which considers both water and air flow in porous materials. The multiphase models have been associated almost exclusively with the petroleum industry. The KANSAS model is a two-dimensional, finite difference approach which uses the alternating direction implicit procedure (ADI) for solution of the equations.

ARCO-IMPES (5C)

The ARCO-IMPES (5C) model is a model used by the Research and Development Department, North American Producing Division of the Atlantic Richfield Company, Dallas, Texas. It is a five component compositional type model for use in three-dimensional gas reservoirs. Since it has five components, there are limits on the number of nodes that can be used. Currently, about 1000 nodes is the largest problem that has been considered in three dimensions. The model utilizes finite differences with an implicit formulation in pressure, but an explicit form in the saturation and saturation dependent characteristics. The user may select between a strongly implicit procedure or a direct method using special ordering and gaussian elimination to solve the difference equations. Though this type of numerical approach would likely perform satisfactorily on the regional type Hanford problems, the compositional features do rather severely restrict the size of problems that can be used.

CONTAMINANT TRANSPORT ANALYSIS

Advection of Conservative Constituents

The simplest models of transport are those which consider only advection. Effectively, only flow kinematics are involved in such

systems, with primary emphasis being on pathlines and their judicious use. There are three potentially useful models of this type.

HANFORD, PCP

The HANFORD, PCP model, better known as the Hanford Pathline Calculation Program, was developed by Dennis Friedrichs of Battelle Northwest for the Groundwater Management Section of the ARHCO Research Department. The calculation program provides a two-dimensional pathline generation capability for use on grided tabular output data from water flow models. It is presently restricted to saturated flow systems with input potential data provided on rectangular grid points for up to 650 data time sets. The spatial potential gradients are obtained using special interpolation expressions that are differentiated and then evaluated. The hydraulic conductivity, effective porosity, and gradient changes with time use direct weighting to obtain the values at the points needed. Though the equal step in time feature is often the more useful mode for following contaminants, the program also can operate in a controlled distance mode along each pathline.

The program was completed recently and has been extensively tested against severe analytical results. Good agreement was found suggesting the PCP model will be a useful evaluation tool for conservative contaminants in two-dimensional flow systems.

FLOP 1 & 2

The FLOP 1 & 2 models are two versions of a Flow Pattern generation capability developed by C. Van Den Akker of the Netherlands Institute for Water Supply. The programs generate numerically the pathlines for two-dimensional flow systems. If analytical potential functions are available, they may be readily incorporated into the programs. However, tabular potential data from measured or numerical solutions from flow models can also be used. The models appear to have been used by more than one technical group in the Netherlands.

FRONT

The FRONT model was developed by A. Vandenberg of the Water Resources Branch of Environment Canada, Ottawa, Ontario, Canada. It performs a two-dimensional simulation of a moving intrusion front in a thin horizontal confined aquifer by predicting the position of a moving interface between contaminated and uncontaminated water. The position of the interface is simulated by following the movements of a finite number of points on the interface for which the initial locations are given on input. This program was designed to run in conjunction with SOPH described earlier, but system flow characteristics could likely be provided by some other flow program with appropriate format adjustments. This model is the only transport model identified under the Advective Changes Only category which predicts a moving front rather than a series of pathlines. The results available from FRONT could be provided by several of the more sophisticated moving particle type transport codes described hereafter by suppressing the dispersion related features.

This completes the strictly flow kinematic models of transport. Other codes of a specialized nature which treat particular flow problems are available, but were not included because of their very special and limited applicability at Hanford. It should also be remembered that some of the models considered in the next section can also be used for direct pathline generation by simply zeroing out the dispersion coefficients or characteristic lengths used for evaluating combined dispersion and advection.

Combined Advection and Dispersive Changes

The next group of transport models combines the effects of advection and dispersion to provide the spatial and time varying distribution of conservative contaminants.

2

INTERA-HCTM

The INTERA-Hydrology Contaminant Transport Model is a coupled model with both conservative contaminant transport capability and the ground-water flow predictive capability (discussed previously) combined into a single computer program. The model provides two- and three-dimensional predictive capability for conservative contaminants. The method of characteristics is used so advection is considered directly through pathlines. The point tracking scheme with dispersion is very effectively utilized in the program. The dispersion characteristics used are a longitudinal and lateral input characteristic length which is automatically combined with the magnitude of effective groundwater pore velocity.

The model has been rather widely applied to a variety of practical problems, which gives it considerable flexibility for general application to different types of problems. Also, since the flow code is so effective, then the coupling of the flow and conservative transport together makes the model an easily run and very useful tool. This efficiency comes from the extensive data manipulation that is saved by the coupled program scheme used. However, since the flow part of the model is restricted to saturated flow, the program is effectively inoperable for use with partially saturated or multiphase flow problems.

SEGOL

The SEGOL model is also a coupled model so transport and flow are solved together.^[26] The flow system is for combined saturated and partially saturated flow as previously discussed, so a more general class of problems can be solved than with the preceding coupled program. The transport equations are solved using a Galerkin Finite Element approach.

USGS, MC

The USGS, MC model was originally formulated by Bredehoeft and Pinder^[33] and has been used extensively by Konikow and others in field

problems.^[34] Though this model has usually been coupled to a flow model, it is so simply separated that it could be utilized alone or directly coupled to another flow model with a minimum of effort. The model considers two-dimensional transport through use of the method of characteristics.

A somewhat unique method is employed in generating the velocity field from groundwater potential data. Central spatial differences are used to estimate gradients at all nodes and at points of contact between node blocks. Values of hydraulic conductivity or transmissivity and porosity at nodes are used directly, while harmonic interpolation provides the hydraulic conductivity values at points between grid node blocks. With the velocities calculated, bilinear interpolation on half grid blocks is used to define the advection components at any point in that half grid space.

Several moving particles are next placed in each cell of the finite difference grid and are moved a distance proportional to the time increment and the velocity at the particle location. The concentration at each node is then temporarily assigned the average concentration of all particles located within that cell. The change in concentration due to dispersion is calculated explicitly for each node, and the average concentration at the node is adjusted for this change. The concentration associated with each particle located in the cell is then adjusted for the node change.

Though potentially useful at Hanford, this model experiences mass balance problems under certain conditions and an improved lagrangian technique is operational on a Hanford computer. However, the specific technique used here to obtain the velocity field could have real utility and may warrant careful consideration.

ISOQUAD

The ISOQUAD model for contaminant transport is a version of ISOQUAD2 where flow and conservative transport are considered together.^[35] This

model utilizes a Galerkin approximation with various basis functions, with a finite element integration scheme to solve the conservative transport equation. The time integration is performed through a backward difference time scheme. The major computer models of this type are presently restricted to considering two-dimensional flow systems. Accordingly, the SEGOL model with potential three-dimensional and combined saturated - partially saturated flow may be a more judicious model to consider for potential Hanford use.

USFLW, Isr.

The USFLW, Isr. model is a combined Unsaturated Flow and contaminant transport model from the group of computer models developed by the Hydrology Division of TAHAL in Israel.

This completes the models considered potentially useful in handling combined advection and dispersion of a conservative subsurface contaminant. The remaining models include the added evaluation capability for chemical and exchangeable reactive constituents.

Contaminant Transport of Reactive Constituents

MMT-DPRW

The MMT or Multicomponent Mass Transport - Discrete Parcel Random Walk model was developed at Battelle Northwest for the Groundwater Management Section of Atlantic Richfield Hanford Company for use in subsurface contaminant flow and other related fluid transport problems.^[36] The generality of the program comes about from the input requirement that the velocity field be an input which is either pregenerated and/or interpolated to the required grid spacing needed by MMT-DPRW for accurate solution. The input velocity field is used to advect discrete parcels along fluid pathlines, i.e., the path where the Lagrangian convection derivative is zero. For this reason, every parcel is independent of every other in the system. Dispersion is next treated through a random walk procedure with appropriate weighting in the longitudinal and transverse flow directions as supplied by the user.

Each parcel is assigned a set of values which correspond to a subdivision of mass of the various chemical species. The developers claim that treating discrete quantities of mass rather than concentrations avoids the mass balance problems associated with several other lagrangian techniques.

The transported and dispersed parcels in a cell together with the liquid volume provide the concentration of each chemical component. From the concentration of each chemical species and the reaction characteristics for every component (both with the soil material and with the other components) the updated chemical composition of the parcels is calculated. The parcels of new chemical composition are then ready for the next sequence of advection, dispersion, and chemical interaction. Such a procedure provides considerable flexibility in incorporating the chemical reaction and interaction characteristics with the porous material into the model. The number of chemical constituents that may be handled by this process is significantly greater than attempting to solve one additional partial differential equation for each new chemical component.

This discrete-parcel-random-walk procedure does require large blocks of computing time to provide solutions, since so many parcels are required in the evaluation. This disadvantage is partially offset by being able to run on smaller, less expensive computers, since the parcel movements are independent of each other. As the model is still early in its development, reductions in run time can be expected. As future computers develop and multiprocessors become available, then such procedures will become much more economical. Also, when considering the cost one must bear in mind that this may be the only feasible way to handle large numbers of chemical components.

SCHWARTZ

The SCHWARTZ model was developed by Franklin W. Schwartz, now of the University of Alberta, Edmonton.^[37] The model uses the method of

characteristics to solve the two-dimensional transport system. The exchange reactions involved binary exchange reactions with the porous material and include radioactive decay in the solution process.

The chemical insight and detailed understanding of chemical exchange reactions with porous materials is most likely of greatest importance in this model.^[38] This is probably more important than potential actual use of the individual model; and such insight might well be incorporated into improved chemical subroutines for the Hanford MMT-DPRW model.

REFQS

The REFQS Model, better known as the Return Flow Quality Simulation Model, was developed in the U. S. Bureau of Reclamation by Marvin J. Shaeffer of the Engineering and Research Center in Denver.^[39] The model was designed to enable evaluating field scale and project-wide consequences of irrigation upon project drainage water quality. It uses a complicated sequence of flow through linear partially saturated columns to the water table, then through the saturated region to a grid drainage network to finally arrive at the fluid outflow. This sequence, though useful for the purpose of evaluating project return flows, is impractical for Hanford use. However, the chemical interactions and exchange approach used could be of significant benefit to the Hanford Groundwater Management Program so the model is included here.

The chemical part of the model simulates many important chemical processes which have been identified and quantified over the years. The particular chemical constituents included in the model are: Ca^{++} , Mg^{++} , Na^{++} , NH_4^+ , NO_3^- , HCO_3^- , CO_3^{--} , Cl^- , SO_4^{--} , urea, organic-N, exchangeable Ca^{++} , Mg^+ , Na^+ , and NH_4^+ and the ion pairs CaSO_4 and MgSO_4 . Equilibrium reactions are predominantly used for most of the inorganic (salt) reactions, but the nitrogen transformations are simulated using kinetic approaches. The approach for handling chemical and exchange reactions, in principle, is the same as used in MMT-DPRW. That is, the constituents are first convected and dispersed, then sequentially chemically reacted at many small time

increments, rather than attempting simultaneous solution of convection, dispersion, and chemical actions on all the constituents when many species must be considered.

OAK RIDGE, FET

The OAK RIDGE Finite Element Transport model was developed by J. O. Duguid and M. Reeves as a two-dimensional companion transport model^[40] for use on the flow results provided by the OAK RIDGE, FE model described previously. The model considers advection, dispersion, and exchange of one chemical constituent which may involve radioactive decay under partially saturated flow conditions. The single chemical component exchange reaction is handled through an equilibrium exchange coefficient modified by the moisture content when partially saturated conditions exist. The spatial integration is accomplished through the Galerkin Finite Element approach using linear basis functions. The time integration uses a modified Crank-Nicholson finite difference form, where the usual differencing location at $\Delta t/2$ is variable in the range from zero to Δt , which the model user may select.

A special, rather standard numbering scheme for element nodes is utilized to reduce the matrix band width that must be stored and operated upon for solution. Special treatment of various boundary conditions are also utilized to maintain the desired matrix forms. The actual solution is standard Gaussian elimination by decomposition into the product of an upper and lower triangular matrices. The lower triangular matrix is used to modify the right hand side for back-substitution into the upper triangular matrix to obtain the solution.

The model is moderately well documented mathematically and very well described as a computer program, including test cases. It would appear that the model being very new has been used only on the two cases illustrated in the document. Experience on a wider range of applications will gradually broaden its scope of significance and flexibility

in use. Only one chemical contaminant can be considered at present, and it appears very difficult, if not impractical, to expand the model to consider additional interacting contaminants.

USFLW, Isr.

The USFLW, Isr. model is an Israeli transport model for use with Unsaturated Flow in materials with contaminants that are sorbed. It uses a method of characteristics solution for the transport equations.

APPENDIX REFERENCES

1. A. O. Gardner, D. W. Peaceman, and A. L. Pozzi, "Numerical Calculations of Multidimensional Miscible Displacement by Method of Characteristics," Society of Petroleum Engineering Journal, March 1964.
2. H. S. Price, and K. H. Coats, "Direct Methods in Reservoir Simulation," Third SPE Symposium on Numerical Simulation of Reservoir Performance of the Society of Petroleum Engineers of AIME at Houston, Texas, January 11-12, 1973, Paper Number 4278.
3. Sumant K. Gupta, Kenneth K. Tanji, and James N. Luthin, "A Three-Dimensional Finite Element Ground Water Model," University of California at Davis Water Resources Center, November 1975.
4. T. N. Naraismhan, and P. A. Witherspoon, "An Integrated Finite Difference Method for Analyzing Fluid Flow in Porous Media," Water Resources Research, February 1976, vol. 12, no. 1.
5. S. P. Neuman, and P. A. Witherspoon, "Analysis of Nonsteady Flow with a Free Surface Using the Finite Element Method," Water Resources Research, June 1971, vol. 7, no. 3, p. 611-623.
6. S. P. Neuman, and P. A. Witherspoon, "Variational Principles for Confined and Unconfined Flow of Groundwater," Water Resources Research, October 1970, vol. 6, no. 5, p. 1376-1382.
7. A. Vandenberg, "Program SOPH - Simulation of Time-Variant Piezometric Surface in a Confined Aquifer Subject to Pumping," Department of the Environment, Ottawa, Ontario, Water Resources Branch, 1974.
8. D. C. Wiggert, "Two-Dimensional Finite Element Modeling of Transient Flow in Regional Aquifer Systems - Analysis of Groundwater Flow in Relation to Water Quality Improvement," Michigan State University, East Lansing, Department of Civil Engineering, August 1974.

9. P. W. France, "Finite Element Analysis of Three-Dimensional Groundwater Flow Problems," Journal of Hydrology, 1974, vol. 21, no. 4, p. 381-398.
10. Peter C. Trescott, "Documentation of Finite-Difference Model for Simulation of Three-Dimensional Groundwater Flow," U. S. Geological Survey Open File Report 75-438, September 1975.
11. H. L. Stone, "Iterative Solution of Implicit Approximations of Multidimensional Partial Differential Equations," Society of Industrial Applied Math, Jour. Numerical Anal., 1968, vol. 5, no. 3, p. 530-558.
12. H. C. Weinstein, H. L. Stone, and T. V. Kwan, "Iterative Procedure for Solution of Systems of Parabolic and Elliptic Equations in Three Dimensions," Indus. Engineering Chemistry Fundamentals, 1969, vol. 8, no. 2, p. 281-287.
13. K. L. Kipp, A. E. Reisenauer, C. R. Cole, and C. A. Bryan, "Variable Thickness Transient Groundwater Flow Model Theory and Numerical Implementation," BNWL-1703, 1972 (Updated 1976), Battelle Pacific Northwest Laboratories, Richland, Washington.
14. R. L. Cooley, "Finite Element Solutions for the Equations of Groundwater Flow," Technical Report Series H-W, Hydrology and Water Resources Publication No. 18, Center for Water Resources Research, Desert Research Institute, University of Nevada System, January 1974.
15. G. F. Pinder, and E. O. Frind, "Application of Galerkin's Procedure to Aquifer Analysis," Water Resources Research, February 1972, vol. 8, no. 1, p. 108-120.
16. G. F. Pinder, "Galerkin-Finite Element Models for Aquifer Simulation," Water Resources Program, Princeton University Princeton, New Jersey, January 1974 (Revised August 1976).
17. T. A. Prickett, and C. G. Lonquist, "Selected Digital Computer Techniques for Groundwater Resource Evaluation," Illinois State Water Survey Bulletin, 1971, vol. 55.

18. P. Armisen, M. Besbes, E. Ledoux, A. Levassor, G. De Marsily, D. Poitrinal, "Sammir: Un Programme Mathematique de Simulation des Aquiferes Multicouches en Mailles Irregulieres sur Ordinateur," Communications presentees au Congres International D'Hydrogeologie, de Porto-Alegre, Bresil, 23-27 Mars 1975.
19. E. M. Weber, "California's Digital Approach to Groundwater Management Studies, "Proceedings - National Symposium on Anal. Water Resource Systems, Denver, Colorado, July 1968.
20. F. A. Rayner, D. M. Wells, B. J. Calborn, D. D. Smith, and A. J. Sechrist, "Mathematical Management Model of Parts of the Ogallala Aquifer, Texas," Final Report, July 1973, High Plains Underground Water Conservation District No. 1, Lubbock, Texas.
21. T. R. Knowles, B. J. Calborn, and D. M. Wells, "A Digital Computer Model for Predicting Regional Aquifer Response," Water Resources Center Report ARC-71-7, December 1971.
22. W. Brutsaert, "Immiscible Multiphase Flow in Groundwater Hydrology: A Computer Analysis of the Well Flow Problem," Ph.D. thesis, Colorado State University, Fort Collins, Colorado, 1970.
23. W. Brutsaert, and C. Way, "A Conjunctive Use Surface Water-Groundwater Simulator," New Mexico Water Resources Research Institute Partial Technical Completion Report No. 033, November 1973.
24. W. F. Brutsaert, "A Functional Iteration Technique for Solving the Richards Equation Applied to Two-Dimensional Infiltration Problems," Water Resources Research, December 1971, vol. 7, no. 6, p. 1583-1595.
25. C.E.K. Rovey, "Numerical Model of Flow in a Stream-Aquifer System," Hydrology Paper No. 74, August 1975.
26. G. A. Segol, "A Three-Dimensional Galerkin Finite Element Model for the Analysis of Contaminant Transport In Variably Saturated Porous Media - Users Guide," June 1976, Department of Earth Sciences, University of Waterloo, Waterloo, Ontario, Canada.

27. M. Reeves, and J. O. Duguid, "Water Movement Through Saturated-Unsaturated Porous Media: A Finite-Element Galerkin Model," ORNL-4927, Contract No. W-7405-eng-26 February 1975, Oak Ridge National Laboratory, Oak Ridge, Tennessee.
28. R. A. Freeze, "Three-Dimensional, Transient, Saturated-Unsaturated Flow in a Groundwater Basin," Water Resources Research, 1971, vol. 7, no. 2, p. 347-366.
29. S. P. Neuman, "Finite Element Computer Programs for Flow in Saturated-Unsaturated Porous Media," Hydrodyn. Hydraul. Lab. Rep. Proj. A10-SEC-77, Technion, Israel Inst. of Technology, Haifa, 1972.
30. S. P. Neuman, "Saturated-Unsaturated Seepage by Finite Elements," Journal of the Hydraulics Division, American Society of Civil Engineers, December 1973, vol. 99, no. HY12, Paper 10201, p. 2233-2250.
31. D. W. Green, C. F. Weinaug, and H. Dabiri, "Numerical Modeling of Unsaturation Groundwater Flow," Kansas Water Resources Research Institute Contrib. 31, Manhattan, Kansas, 1969.
32. D. W. Green, H. Dabiri, and C. F. Weinaug, "Numerical Modeling of Unsaturation Groundwater Flow and Comparison of the Model to a Field Experiment," Water Resources Research, June 1970, vol. 6, no. 3, p. 862-874.
33. J. D. Bredehoeft, and G. F. Pinder, "Mass Transport in Flowing Groundwater," Water Resources Research, 1973, vol. 9, no. 1, p. 194-209.
34. Leonard F. Konikow, and John D. Bredehoeft, "Modeling Flow and Chemical Quality Changes in an Irrigated Stream-Aquifer System," Water Resources Research, June 1974, vol. 10, no. 3, p. 546-562.
35. George F. Pinder, "A Galerkin - Finite Element Simulation of Groundwater Contamination on Long Island, New York," Water Resources Research, December 1973, vol. 9, no. 6, p. 1657-1669.

36. S. W. Ahlstrom and H. P. Foote, "Multicomponent Mass Transport-Discrete Parcel Random Walk Model Theory and Numerical Implementation," BNWL-2127, Battelle Pacific Northwest Laboratories, to be published December, 1976.
37. Franklin W. Schwartz, "On Radioactive Waste Management: An Analysis of the Parameters Controlling Subsurface Contaminant Transfer," Journal of Hydrology, 1973, vol. 27, p. 51-71.
38. Franklin W. Schwartz, and Patrick A. Domenico, "Simulation of Hydrochemical Patterns in Regional Groundwater Flow," Water Resources Research, June 1973, vol. 9, no. 3, p. 707-720.
39. Marvin J. Shaffer, and Richard W. Ribbens, "Generalized Description of Return Flow Quality Simulation Model," Engineering and Research Center, Bureau of Reclamation, October 1974, U. S. Department of Interior, Denver, Colorado.
40. J. O. Duguid, and M. Reeves, "Material Transport Through Porous Media: A Finite Element Galerkin Model," ORNL-49280, March 1976, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

ACKNOWLEDGMENTS

The authors express their thanks to Messrs. J. R. Eliason, J. R. Raymond and S. W. Ahlstrom of Battelle, Pacific Northwest Laboratories for helpful suggestions and review of sections of the final manuscript. Appreciation is also extended to Ms. Juanita Cole of Atlantic Richfield Hanford Company and the Battelle technical typing team lead by Ms. Barbara Haner for their considerable effort in typing the many drafts of this report.

DISTRIBUTION

OFFSITE

Energy Research and Development
Administration Technical
Information Center (285)

Ronald L. Bullard
Chief, Environmental
Specialist Branch
Nuclear Regulatory Commission
Directorate of Regulation
7920 Norfolk Avenue
Bethesda, MD 20014

W. Gamill
Chief, Site Analysis Branch
Nuclear Regulatory Commission
Directorate of Regulation
7920 Norfolk Avenue
Bethesda, MD 20014

D. E. Saire
Waste Management Production
and Reprocessing
Washington, D.C. 20545

Dr. Adrian H. Dahl
Chief, Environmental Science
Branch
Energy Research and Development
Administration
Idaho Falls, ID 83401

Dr. Leo Heindl
Executive Secretary
National Academy of Science
U.S. National Committee for the
IHD
2101 Constitution Avenue
Washington, D.C. 20418

Technical Secretary
National Academy of Science
Committee on Radioactive Waste
Management
National Research Council
2101 Constitution Avenue
Washington, D.C. 20418

Dr. K. L. Kipp
AERE Harwell
Oxfordshire, England

Marvin J. Shaffer
U.S. Department of the Interior
Bureau of Reclamation
Engineering and Research Center
Federal Center
Denver, CO 80225

Merlin Wheeler
Division H8
Environmental Studies
Los Alamos Scientific Laboratory
Los Alamos, New Mexico

J. O. Duguid
Environmental Sciences Division
Union Carbide Corporation
Oak Ridge National Laboratory
Oak Ridge, TN 37830

D. L. Shaeffer
Environmental Sciences Division
Union Carbide Corporation
Oak Ridge National Laboratory
Oak Ridge, TN 37830

G. A. Segol
Canadian Bechtel Limited
250 Blour Street East, Suite 1600
Toronto, Ontario M4W 3K5
CANADA

P. W. France
Department of Civil Engineering
and Building Technology
University of Wales
Institute of Science and Technology
Cardiff, Great Britain

D. B. McWhorter
Department of Agricultural Engineering
Colorado State University
Fort Collins, CO 80523

D. C. Wiggert
Department of Civil Engineering
Michigan State University
East Lansing, MI

Chris Wheeler
State Engineer
State of Oregon
516 Public Service Bldg.
Salem, OR 97310

C. Stephen Allred
Deputy Director
Department of Water Resources
Annex 2 Statehouse
Boise, ID 83720

J. W. Keely
Chief, Subsurface Environmental
Research Branch
Robert S. Kerr Research Lab
P.O. 1198
Ada, OK 74820

Thomas A. Prickett
Engineer
Illinois State Water Survey
Box 232
Urbana, IL 61801

Dan Wiersma
Director, Water Resources Research
Center
Lilly Hall of Life Science
Purdue University
South Bend, IN

Jacob Bear
Professor, Vice President for
Academic Affairs
Department of Civil Engineering
Technion, Israel Inst. of
Technology
Haifa, Israel

Keros Cartwright
Geologist and Head
Hydrogeology and Geophysics
Section
Illinois State Geological Survey
Urbana, IL 61801

E. O. Frind
Assistant Professor
Department of Earth Sciences
University of Waterloo
Waterloo, Ontario
CANADA

C. S. Desai
Professor
Department of Civil Engineering
V.P.I. and S.U.
Blacksburg, VA 24061

R. A. Freeze
Associate Professor
Department of Geology
University of British Columbia
Vancouver, B.C.
CANADA

Dr. Frank L. Parker
Vanderbilt University
Nashville, TN 37203

D. Kirkham
Iowa State University
Ames, IA

G. F. Pinder
Princeton University
Department of Civil and Geological
Engineering
Princeton, NJ 08540

Professor Ven Te Chow
Hydrosystems Laboratories
University of Illinois
Urbana, IL 61801

James Crosby, III
Geologist
Washington State Water Research
Center
Pullman, WA 99163

Technical Secretary
National Academy of Science
Committee on Radioactive Waste
Management
National Research Council
2101 Constitution Avenue
Washington, D.C. 20418

George Debuchananne
Director
U.S. Geological Survey
2100 M. Street
Washington, D.C. 20037

J. D. Bredehoeft
U.S. Geological Survey
Water Resources Division
Reston, VA 22092

P. C. Trescott
U.S. Geological Survey
Water Resources Division
Reston, VA 22092

P. A. Witherspoon
Department of Civil Engineering
University of California
Berkeley, CA 94720

J. N. Luthin
University of California at Davis
Department of Water Sciences and
Engineering
Davis, CA 95616

W. H. Brutsaert
Cornell University
School of Civil Engineering
B22 Bailey Hall
Ithaca, NY 14850

Dr. Larry Boersma
Professor of Soils
Oregon State University
Corvallis, OR 97331

P. J. Wierenga
New Mexico State University
Department of Agronomy
P.O. Box 30
Las Cruces, New Mexico 88001

Eugene Wallace
Supervisor Water Resources Division
State of Washington
Department of Ecology
Olympia, WA 98501

R. B. Lantz
Executive Vice-President
Intera Environmental Consultants
1201 Dairy Ashford, Suite 200
Houston, TX 77079

Sumant K. Gupta
Department of Land, Air and Water
Resources
University of California
Davis, CA 95616

Shlomo P. Neuman
Hydrology and Water Resources Department
University of Arizona
Tucson, AR

A. Vandenberg
Water Resources Branch
Inland Waters Directorate
Environment Canada
Ottawa, KIA-0E7
Ontario, CANADA

J. Schwarz
Head, R&D Section
Hydrology Division Tahal
P.O. Box 11170
Tel Aviv, Israel

Frank W. Schwartz
Assistant Professor
Department of Geology
University of Alberta
Edmonton, CANADA

E. S. Simpson
Professor
Department Hydrology and Water
Resources
University of Arizona
Tucson, AZ 85721

Georges Vachaud
Maitre de Recherches
Institut de Mécanique de Grenoble
USMG - BP53
F 38041-Grenoble Cedex France

C. Van Den Akker
Hydrologist
Municipal Water Works of Amsterdam
Condensatorweg 54
Amsterdam/Sloterdijk
The Netherlands

L. F. Konikow
U.S. Geological Survey
Building 53
Federal Center
Denver, CO

D. Grove
U.S. Geological Survey
Building 53
Federal Center
Denver, CO

R. L. Cooley
U.S. Geological Survey
Building 53
Federal Center
Denver, CO

Harvey O. Banks
Consulting Engineer
3 Kittie Lane
Belmont, CA 94002

Patrick Domenico
Department of Geology
University of Illinois
Urbana, IL 61801

Erik Eriksson
Department of Physical Geography
University of Uppsala
Box 554
S-751 22 Uppsala 1
Sweden

German E. Figueroa Vega
Director de Aguas Subterráneas
Y Superficiales
Comision de Aguas del Valle de Mexico
Balderas 55
Mexico, D.F.

Luis Lopez Garcia
INTECSA
Apartado 13104
Condesa de Venadito 1
Madrid 27, Spain

Pavel Koryavov
Computation Center
Academy of Sciences
40 Vavilov Street
Moscow 11733, U.S.S.R.

Ghislain de Marsily
Directeur de Centre d'Informatique
Geologique
Ecole Nationale Supérieure
des Mines de Paris
35, Rue Saint-Honore
77305 Fontainebleau
France

George Burke Maxey
Director
Center for Water Resources Research
Desert Research Institute
University of Nevada
Reno, Nevada 89507

Jerome Milliman
Department of Economics
University of Florida
Gainesville, Florida 32601

John R. Philip, Chief
Division of Environmental Mechanics -
CSIRO
P.O. Box 821
Canberra City A.C.T. 2601
Australia

Jehoshua Schwarz
Tahal - Consulting Engineering Ltd.
P.O. Box 11170
Tel Aviv, Israel

Tatsuo Shibasaki
Consulting Geologist
Group Leader of Research Group
for Water Balance
182 Fujigane
Tsurugashima, Saitama 350-02
Japan

Robert G. Thomas
Senior Officer (Water Resources)
Land and Water Development Division
Food and Agriculture Organization
of the United Nations
Via delle Terme di Caracalla
00100 - Rome
Italy

John Wilson
Parsons Laboratory for Water
Resources and Hydrodynamics
Department of Civil Engineering
Building 48-209
Massachusetts Institute of Technology
Cambridge, MA 02139

Francois N. Frenkiel
Computation and Mathematics Department
Naval Ship Research and Development
Center
Bethesda, MD 20084

Thomas F. Malone
Director
Holcomb Research Institute
Butler University
Indianapolis, IN 46208

Ted Munn
Atmospheric Environment Service
4905 Dufferin Street
Downsview, Ontario
Canada N3H 5T4

Yehuda Bachmat
Project Director
Holcomb Research Institute
Butler University
Indianapolis, IN

ONSITE

Battelle-Northwest
DB Cearlock
HC Burkholder
JR Eliason
AE Reisenauer

Battelle-Northwest (Cont')

CR Cole (2)
DR Friedrichs
SW Ahlstrom
GW Dawson
KM Harmon
AK Tyagi
JR Raymond

United Nuclear Inc.
AL Cucchiara

Westinghouse Hanford Company
RB Hall

ERDA Richland Operations Office
OJ Elgert
JL Rhoades
PG Rhoades
RB Goranson
GJ Bracken

Atlantic Richfield Hanford Company
RC Arnett (30)
H Babad
DJ Brown
RA Deju (4)
PA Eddy
PG Easley
RD Fox
RE Gephart
RE Isaacson
RK Ledgerwood
MW Legatski
WH Riggsbee
HP Shaw
ARHCO Document Control (2)