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SELECTION CRITERIA FOR MATHEMATICAL MODELS USED IN EXPOSURE ASSESSMENTS: GROUND-WATER MODELS

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FOREWORD

When performing exposure assessments using predictive methods, assessors frequently ask the following questions: "How do I select the best fate model to use in my assessment," "How can I tell if the model someone else used in their assessment is appropriate," and "What are the strengths and weaknesses of these models?" This document is a first step in addressing these questions.

One of the functions of the Exposure Assessment Group is to develop guidelines for exposure assessments. On September 24, 1986, the U.S. Environmental Protection Agency published Guidelines for Estimating Exposures. During the development of the guidelines and subsequent review and comment, four areas were identified that required further research. One of these areas was selection criteria for mathematical models. This document, which is the second selection criteria document in the series, deals with ground-water models. The first dealt with surface water models. Similar documents will follow dealing with air models, and int he future, other types of models.

This document is designed to help the exposure assessor evaluate the appropriateness of models for various situations. The report defines the terms and discusses the general approaches that modelers take to a problem so that exposure assessors may more readily evaluate the appropriateness of both new and existing models. In addition, step-by-step criteria are provided to enable the assessor to answer the questions posed above.

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PREFACE

The Exposure Assessment Group of the Office of Health and Environmental Assessment (OHEA) is preparing several documents addressing selection criteria for mathematical models used in exposure assessments. These documents will serve as technical support documents for the Guidelines for Estimating Exposures, one of five risk assessment guidelines published by the U.S. Environmental Protection Agency in 1986.

The purpose of this document is to present criteria which provide a means for selecting the most appropriate mathematical model(s) for conducting an exposure assessment related to ground-water contamination.

The literature search to support the models discussed in this report is current to September 1986.

ABSTRACT

Prior to the issuance of the Guidelines for Estimating Exposures in 1986, the U.S. Environmental Protection Agency (EPA) published proposed guidelines in the Federal Register for public review and comment. The purpose of the guidelines is to provide a general approach and framework for carrying out human and nonhuman exposure assessments for specific pollutants. As a result of the review process, four areas were identified that required further research. One of these was the area of selection criteria for mathematical models used in exposure assessments.

The purpose of this document is to present criteria which provide a means for selecting the most appropriate mathematical model(s) for conducting an exposure assessment related to ground-water contamination.

General guidelines and principles for model selection criteria are presented followed by a step-by-step approach to identifying the appropriate model(s) for use in a specific application. Several of the currently-available models are grouped into categories and a framework is provided for selecting the appropriate model(s) based on the response to the technical criteria. Brief summaries of all the currently available models discussed in this report are contained in the appendix.

Two site-specific example problems are provided to demonstrate the procedure for selecting the appropriate mathematical model for a particular application.

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1. EXECUTIVE SUMMARY

1.1. INTRODUCTION

This document presents a set of criteria which provide a means of selecting the most appropriate mathematical model for conducting an exposure assessment related to ground-water contamination. These criteria were developed in recognition of the growing use of exposure assessments across the U.S. Environmental Protection Agency's regulatory programs. Use of the criteria will expedite the regulatory process by eliminating the use of unacceptable or inappropriate models. Their use will also improve the quality of data used in the decision-making processes and promote consistency in exposure assessments.

When performing a predictive exposure assessment, a major task is to predict the transport of contaminants. Since ground-water flow is an integral part of contaminant transport, it is equally important, if not more so, to accurately predict the ground-water flow. Therefore, both ground-water flow and contaminant transport mathematical models, and criteria for selecting these models, are discussed in this document.

1.2. BACKGROUND INFORMATION

Some of the general background information necessary to understand the selection of a ground-water flow and/or contaminant transport model is discussed in this section. This chapter is intended for the exposure assessor or the non-modeler who is not completely familiar with hydrogeologic and modeling terms.

The first section provides a primer on ground-water flow. The intent of this section is to provide a brief summary of the background information necessary to understand ground-water problems. The chapter discusses the

general terms used to describe and define ground-water flow and presents the basic equation for flow in a ground-water system.

The second section provides background information on contaminant transport in ground water. The chapter presents the basic equation for advective-dispersive transport and discusses the important terms in detail.

The last section provides definitions for terms used throughout the report.

1.3. GENERAL GUIDELINES AND PRINCIPLES OF MODEL SELECTION CRITERIA

In order to enhance understanding and facilitate implementation of the mathematical model selection criteria, the following terms are defined: mathematical model, process equation, analytical solution, analytical models, numerical models, objectives criteria, technical criteria, and implementation criteria. The relationship between these terms may be thought of as follows. A mathematical model consists of two aspects: a process equation and a solution technique to solve the process equation. An analytical solution solves a very simple process equation analytically by hand calculations. An analytical model solves a more complex, but still relatively simple, process equation analytically with a computer program. A numerical model solves a simple or complex process equation numerically with a computer program. In the context of this document, mathematical model refers to all three solution techniques of a process equation. The more detailed the specific application, the more complex the process equation. The complexity of the process equation dictates the solution technique required.

There are three factors which dictate the level of complexity of the mathematical model chosen in the selection process:

1. objectives criteria;
2. technical criteria; and

3. implementation criteria.

The objectives criteria refer to the level of modeling detail required to meet the objectives of the study. There are many different objectives of modeling studies, however, in the context of model selection, all objectives are classified in two broad categories: 1) to perform a screening study or 2) to perform a detailed study.

A screening study is one where the purpose is to make a preliminary screening of a site or to make a general comparison between several sites. A detailed study, on the other hand, is one where the objective is to make an assessment of the environmental impact, performance, or safety of a specific site.

Based on the objectives of the study (screening or detailed levels), the analyst or modeler will select either a screening or detailed model. The specific model to be used will be selected based on the technical selection criteria discussed below.

1.3.1. Technical Criteria

The second level of consideration when selecting a mathematical model is the technical criteria. Technical criteria are those criteria related to the mathematical model's ability to simulate the site-specific contaminant transport and fate phenomena of importance.

With regard to model selection, the technical criteria can be divided into three categories:

1. transport and transformation processes;
2. domain configuration; and
3. fluid(s) and media properties.

Transport and transformation process criteria relate to those significant processes or phenomena known to occur on site that must be modeled in order to properly represent the site. Domain configuration relates to the ability of the model to accurately represent the geohydrologic system. When high levels of resolution are required to predict contaminant concentrations for comparison to health or design standards, it is generally necessary to simulate site-specific geometry and dimensionality for which numerical models are most appropriate. If simplifying the site geometry can be defended on a geologic and hydrologic basis, then the use of a simpler analytical model/solution may be justified. The third category of technical criteria corresponds to the ability of the mathematical model to represent the spatial variability of fluid(s) and media properties of the geohydrologic site.

Once the level of model has been decided, the technical criteria will direct the analyst to the specific type of model needed to properly simulate the transport and transformation aspects of the environmental setting.

1.3.2. Implementation Criteria

The third level of consideration when selecting a mathematical model is related to the implementation criteria. Implementation criteria are those criteria dependent on the ease with which a model can be obtained and its acceptability demonstrated. Whereas the technical criteria identify the models capable of simulating the relevant phenomena within the specified environmental setting, the implementation criteria identify documentation, verification, validation requirements, and ease of use so that the model selected provides accurate, meaningful results.

1.3.3. Other Factors Affecting Model Selection

Other general factors related to model selection which are secondary to the technical or implementation criteria include data availability, schedule, budget, staff and equipment resource, and level of complexity of system(s) under study. Schedule and budget constraints refer to the amount of time and money available for the assessment. If both analytical and numerical models meet the selection criteria, time and cost may be considered factors for electing to use an analytical approach.

1.4. MODEL SELECTION DECISION PROCESS

The decisions to be made when selecting a ground-water flow model are discussed in detail in this section. Some guidance is provided for making the decision and some discussion is provided regarding the errors associated with using the incorrect model or feature(s) of a model. The criteria for ground-water flow are presented followed by those for contaminant transport.

- Are you simulating a water table (i.e., unconfined) or a confined aquifer, or a combination of both (i.e., conditions change spatially)?
- Does the ground water flow through porous media, fractures, or a combination of both?
- Is it necessary to simulate three-dimensional flow or can the dimensionality be reduced without losing a significant amount of accuracy?
- Are you simulating a single-phase (i.e., water) or a multi-phase (i.e., water and oil) flow system?
- Can the system be simulated with a uniform value (homogeneous) or spatially variable values (heterogeneous) of hydraulic conductivity, porosity, recharge, and/or specific storage?

- Is there a single or are there multiple hydrogeologic layers to be simulated?
- Is (are) the hydrogeologic layer(s) of constant or variable thickness spatially?
- Is the hydrologic system in a steady-state condition or do water levels fluctuate with time (transient condition)?

After all these criteria has been satisfied, in most cases there will be several ground-water flow models which would be appropriate. At this point the analyst can either select a ground-water flow model and then continue with the selection process to select a compatible (but separate) contaminant transport model, or the user can continue the process to select a combined flow and transport model. It is quite common to develop a fairly sophisticated flow model to predict ground-water travel paths and velocities and link it with a simpler transport model.

The decisions to be made when selecting a contaminant transport model are discussed in detail in this section. Some guidance is provided to help in making the decision and some discussion is provided regarding the errors associated with using the incorrect model or feature(s) of the model.

- Does the contaminant enter the ground-water flow system at a point or is it distributed along a line or over an area or a volume?
- Does the source consist of an initial slug of contaminant or is it constant over time?
- Is it necessary to simulate three-dimensional transport or can the dimensionality be reduced without losing a significant amount of accuracy?
- Does the model simulate dispersion?

- Does the model simulate adsorption (i.e., distribution or partitioning coefficient) and, if so, does it simulate temporally and/or spatially variable adsorption? Temporally or spatially variable adsorption is important where the soil conditions and/or concentrations change with time and space.
- Does the model simulate first or second-order decay and/or radionuclide decay?
- Does the model simulate density effects related to changes in temperature and concentration? A truly coupled model is one where the ground-water flow is influenced by the density and viscosity of the water, which are influenced by the temperature of the water and the concentration of the solute. In some cases (i.e., large heat source or large fluctuations in solute concentration) it may be important to consider temperature and contaminant concentration effects on ground-water flow.

After sequencing through the decision tree, there will, in most cases, be several models which meet the desired criteria. Since several models could meet the desired criteria, it is difficult to list a single model as a standard model. At this point the analyst can either select a transport model which is compatible with the flow model selected above, or select a combined ground-water flow/contaminant transport model.

Regardless of the approach selected, separate or combined flow and transport model, it is likely that there will be several models which meet the technical criteria. The selection of the final model(s) should be based on the implementation criteria, i.e., the model has been through a rigorous quality assurance program so that it is thoroughly verified and the model is well documented with user's manuals and test cases.

If several models pass the quality assurance and documentation criteria, the final selection of a model should be based on familiarity with and availability of the model, schedule, budget, and staff and equipment resources.

A model selection worksheet is included in this section which facilitates the selection of the actual model or suite or models to be used based on the response to the technical criteria. Separate worksheets are provided for both analytical solutions and for analytical and numerical models (coded for the computer). A summary of each of the models contained in the worksheets is contained in Appendix A.

A discussion of waste management models has been included in this section. Waste management models are defined as models which trace contaminant movement through the three primary environmental pathways: air, surface water, and/or ground water. It is not the objective of this document to cover waste management models in any detail. Rather, a few such models are described briefly to make the reader aware of them. The models discussed are:

1. risk assessment methodology for regulatory sludge disposal through land application;
2. risk assessment methodology for regulating landfill disposal of sludge;
3. RCRA risk/cost policy model (WET model);
4. the liner location risk and cost analysis model; and
5. landfill ban model.

1.5. MODEL SELECTION EXAMPLE PROBLEMS

Two site-specific example problems are provided in this section to demonstrate the procedure for selecting the appropriate mathematical model for a particular application. The first example is an application where the objective is to perform a screening study, while the objective of the second example is to

perform a detailed study. The discussions of the example problems are presented in the order that should be followed when conducting a ground-water flow and contaminant transport model study, with model selecting being one element of the process.

1.6. APPENDIX A

The appendix of the document contains a summary page for each of the analytical and numerical mathematical models discussed in Table 5-3. The models are divided into seven categories:

1. analytical flow models;
2. analytical transport models;
3. numerical flow models which can be applied to both saturated and unsaturated systems;
4. numerical flow models which can only be applied to saturated systems;
5. numerical contaminant transport models which can be applied to both saturated and unsaturated systems;
6. numerical contaminant transport models which can only be applied to saturated systems; and
7. numerical contaminant and heat transport models which couple the solutions for pressure, temperature, and concentration (coupled models).

2. INTRODUCTION

This document presents a set of criteria which provide a means of selecting the most appropriate mathematical model for conducting an exposure assessment related to ground-water contamination. These criteria were developed in recognition of the growing use of exposure assessments across the U.S. Environmental Protection Agency's regulatory programs. Use of the criteria will expedite the regulatory process by eliminating the use of unacceptable or inappropriate models. Their use will also improve the quality of data used in the decision-making processes and promote consistency in exposure assessments.

These selection criteria are particularly directed toward exposure assessments. However, the same or very similar criteria would be applicable to all aspects of managing ground-water contamination problems/sites. To manage contamination problems/sites, mathematical models are needed to perform initial screening studies, assist in the design of disposal schemes, assess the probable contaminant performance of specific sites, predict contaminant migration, and aid in the design of monitoring programs and remedial action alternatives.

In the context of this document, the term mathematical model refers to both analytical and numerical solutions. Analytical solutions refer to both those which are coded for the computer as well as those which are suitable for hand calculation. Numerical solutions refer only to those which are coded for solution on the computer since this is the only practical solution technique. Throughout most of the report, the term mathematical model is shortened simply to model.

When performing an exposure assessment, the primary interest is in predicting the transport of contaminants. However, since ground-water flow is

an integral part of contaminant transport, it is equally important, if not more so, to accurately predict the ground-water flow. Therefore, both ground-water flow and contaminant transport mathematical models, and criteria for selecting these models, are discussed in this document. Related models, such as unsaturated flow, nonaqueous phase liquid, and geochemical models, are not discussed in this document.

In order to develop a tractable, useful model, the importance of the various processes controlling contaminant migration in ground water must be identified. Only the dominant processes are incorporated in the mathematical models. The explicit incorporation of every known or observed process is not practical because the resulting model would require excessive computational time and would contain too many internal coefficients that must be adjusted in the calibration or initial phase of a modeling study. In addition, the effect of the minor processes, in terms of the predicted concentration levels, is very small in comparison with the dominant transport processes and attenuation mechanisms.

All of the contaminant transport models discussed in this report are designed for situations where the contaminant is at trace concentration levels. Trace concentrations, in this context, are defined as concentrations that have a negligible impact on the density and viscosity of the fluid and, therefore, have an insignificant effect on the ground-water movement. The models are not designed to be used in an emergency response framework, such as an accidental spill, because in those situations 1) the contaminant is not likely to be at trace concentrations initially and 2) the time required to set up the model, run the model, and evaluate results is generally greater than the emergency response times.

This document is intended primarily to assist potential model users who are not experts in water quality modeling. A concerted effort has been made to define specific terminology and to characterize the important assumptions and limitations of the existing models. The existing models are generally the best available technology and are useful tools when applied properly. However, model accuracy is very sensitive to input parameters and calibration with field data is essential. In any modeling study the assumptions and limitations of a particular model along with the means by which it is applied should be clearly understood by the model user as well as by persons making decisions based, in part, on the modeling results. Although the guidance provided in this document is primarily directed toward applications-oriented users of mathematical models, the information presented is also important to managers and other decision makers who will have the ultimate responsibility of assessing and controlling contamination problems.

In view of the diversity in typical modeling needs and objectives associated with exposure assessments and related studies, these selection criteria are formulated as a general guideline for selecting a relevant or appropriate mathematical model. They are not intended to serve as an absolute set of standards for accepting or rejecting models for possible use in exposure assessments.

These criteria deal only with the selection of existing mathematical models for predicting ground-water flow and contaminant transport. The criteria do not deal with the development of numerical algorithms for constructing new models. Two other reports which address the issue of model selection criteria are Simmons and Cole, 1985, and U.S. EPA, 1987.

The organization of this document is as follows:

Chapter 2 -- Background Information -- General discussion of ground-water flow and contaminant transport, description of equations and processes, and definition of specific terms.

Chapter 3 -- General Guidelines and Principles of Model Selection Criteria -- Overview of the modeling process, overview of model selection criteria, and important issues related to model selection.

Chapter 4 -- Model Selection Decision Process -- Step-by-step process to identify the appropriate model(s) for a specific application.

Chapter 5 -- Model Selection Example Problems -- Examples of how to use the selection criteria.

Appendix A -- Analytical and Numerical Model Summaries.

3. BACKGROUND INFORMATION

Some of the general background information necessary to understand the selection of a ground-water flow and/or contaminant transport model is discussed in this section. This chapter is intended for the exposure assessor or the non-modeler who is not completely familiar with hydrogeologic and modeling terms. It should be emphasized that the information presented here is a brief overview. For much more detailed discussions the reader is directed to the following sources: Freeze and Cherry, 1979; Chow, 1964; Davis and DeWest, 1966; Javandel et al., 1984; Bachmat et al., 1980, and Mercer and Faust, 1981.

The first section provides a primer on ground-water flow. The second section provides background information on contaminant transport in ground water. The last section provides definitions for terms used throughout this report.

3.1. PRIMER ON GROUND-WATER FLOW

This section is intended to provide a brief summary of the background information necessary to understand a ground-water problem. The chapter discusses the general terms used to describe and define ground-water flow and presents the basic equation for flow in a ground-water system.

3.1.1. Ground Water and the Hydrologic Cycle

The hydrologic cycle can be defined as the endless circulation of water between ocean, atmosphere, and land. The hydrologic cycle is composed of precipitation, storage, runoff, and evaporation of the earth's water during the cycle. The total amount of water is essentially fixed, but its form may change (i.e., solid, liquid, gas).

Our interest for the purposes of this report is in the land-based portion of the cycle, particularly the portion that infiltrates the land surface and flows underground. The subsurface distribution of water can be divided into five categories:

1. Soil Zone -- That area where evaporation and transpiration of water occurs (partially saturated).
2. Vadose (Unsaturated) Zone -- Partially-saturated zone consisting of sediments whose interconnected pore space (porosity) is not completely filled with water. Water flow in this region can be both horizontal and vertical as stratification of the sediments will cause significant conductivity contrasts.
3. The Capillary Fringe -- A transition zone from the partially-saturated vadose zone to the fully-saturated phreatic (water table) surface.
4. Phreatic (Saturated) Zone -- Below the phreatic surface, the porous material is fully saturated with water (with the exception of entrapped gas). Water in this zone is under hydrostatic pressure. The porous material is called the aquifer.
5. Dense Rock -- The phreatic zone merges at depth into a zone of dense rock with water in the pore spaces but few or none of these pore spaces are interconnected and flow of water is severely limited.

That portion of the hydrologic cycle beneath the land surface can be called the subsurface flow system. Inflow or recharge to the subsurface flow system arrives as precipitation (in the form of rainfall or snowmelt) or as infiltration from surface water bodies. Outflow or discharge occurs as evapotranspiration or evaporation and as flow to surface water bodies. Artificial recharge and discharge occur as injection or pumping, respectively.

In this report, the selection of models developed to simulate ground-water flow and contaminant transport in the saturated zone is discussed in detail. Therefore, the rest of this background discussion is directed to flow in the phreatic or saturated zone.

Water that infiltrates the land surface generally moves vertically downward to the water table and the phreatic zone. Water in the phreatic zone generally moves horizontally from areas of greater to areas of lesser hydrostatic head (i.e., energy: see Section 3.1.3). In both zones, unsaturated and saturated, the prime moving force is gravity.

The occurrence, movement, and storage of ground water are related to and influenced by the porous media structure, lithology, thickness, hydraulic conductivity, hydraulic gradient, and porosity. A formation, or group of formations, that contains sufficient saturated permeable material to yield significant quantities of water to wells and springs is defined as an aquifer. Movement and storage of water in an aquifer are chiefly controlled by the aquifer hydraulic conductivity, permeability, and porosity. Aquifers can be subdivided into three main types as follows:

1. Unconfined (Water Table) Aquifer -- An aquifer in which the top of the saturated zone (water table) is in direct contact with the atmosphere through the open pores of the earth material above.
2. Confined (Artesian) Aquifer -- An aquifer which has an overlying layer which does not allow direct contact of the aquifer with the atmosphere. Water in a confined aquifer is under pressure and wells penetrating into the aquifer will have a water level that reflects the pressure in the aquifer at the point of penetration.

3. Perched Aquifer -- Beds of clay or silt or other materials of limited areal extent which present a restriction to flow of downward moving water in the vadose zone may cause local areas of saturation above the regional water table. An unsaturated zone is present between the bottom of the perching bed and the water table.

Aquifers have a higher hydraulic conductivity than adjacent units. The lithologic units of low hydraulic conductivity relative to the aquifer are commonly called aquitards. Appreciable quantities of water can move through an aquitard, in most cases vertically upward and/or downward, from aquifers above and below. If very little flow occurs, the unit is termed an aquiclude.

3.1.2. Porosity and Hydraulic Conductivity

The portion of an aquifer's volume which consists of openings or pores and not solid material is defined as porosity. Porosity is an index of how much water can be stored in the saturated material and is usually expressed as a percentage of the bulk volume of the material. Effective porosity is defined as the ratio of the transmissive pore volume to the total unit volume, where the transmissive pore volume is that portion which contributes to the net flow through the system.

Hydraulic conductivity (K) is a measure of the capacity of a porous rock, soil, or sediment to transmit water. Aquifers having high hydraulic conductivity generally consist of clean coarse sands and mixtures of sand and gravel and fine sands, silts, or clays. Aquifers having low hydraulic conductivity generally consist of very fine sands, silts, and clays, glacial till, or stratified clays.

Average values of hydraulic conductivity for different soil classes are as follows:

Soil Class	Hydraulic Conductivity (cm/sec)	(gpd/ft^2)
Clay	10^{-6}-10^{-3}	10^{-2}-10
Sand	10^{-3}-1.0	10 -10^4
Gravel	1.0 -10^2	10^4 -10^6

If a hydraulic conductivity is independent of position in an aquifer, the formation is homogeneous. If the conductivity is dependent on position, the formation is heterogeneous (i.e., K varies from point to point in the medium). If the conductivity is independent of the direction of measurement at a point in the aquifer, the formation is isotropic at that point. If conductivity varies with the direction of measurement at a point in an aquifer, the formation is anisotropic at that point. A formation can be isotropic and heterogeneous, which is not at all uncommon. Anisotropy is common when the conductivity varies in the x (horizontal) and z (vertical) direction. In many aquifers the vertical conductivity can be estimated as one tenth the horizontal conductivity.

The transmissivity of an aquifer is defined as the rate at which water of the prevailing kinematic viscosity is transmitted through a unit width under a unit hydraulic gradient. Though spoken of as a property of the aquifer, it embodies also the saturated thickness and the properties of the contained liquid. Transmissivity is also defined as the product of hydraulic conductivity and aquifer thickness.

The storage coefficient of an aquifer is defined as the volume of water released from storage in a vertical column of 1.0 square feet when the water table or other piezometric surface declines 1.0 feet. In an unconfined aquifer, it is approximately equal to the specific yield, which is defined as the amount of water that drains from a soil due to the force of gravity.

3.1.3. Flow in Ground-Water Systems

In 1856 Henry Darcy reported that flow between two points in a soil column is directly proportional to the difference in potential head (energy) between the points and inversely proportional to the distance between the points. These two quantities together (difference in head divided by the distance between the points) are known as the hydraulic gradient. Darcy's Law can be written as

$$Q = -KA\,(h_1-h_2)/L \qquad (3\text{-}1)$$

where Q = flow rate (L^3/t)

K = permeability or hydraulic conductivity of the media and fluid (L/t)

A = cross-sectional area of flow (L^2)

h_1, h_2 = potential head at two points on a line parallel to flow (L)

L = length of flow path from h_1 to h_2 (L)

h_1-h_2/L = hydraulic gradient = head drop per unit distance

The negative sign in Equation 3-1 indicates that ground-water flows from high to low potential. Head, potential, fluid potential, and potential head are all the same and can be defined as the mechanical energy per unit mass of a fluid at any given point in space and time with respect to an arbitrary state and datum (typically mean sea level).

Darcy's Law is valid for steady flow with constant flux. The law is only valid for laminar flow, not when the flow becomes turbulent which is not common in ground water. Darcy's Law is a measure of the average or bulk velocity through a given cross section of a porous medium. The true ground-water velocity between soil grains is defined as the Darcy velocity divided by the porosity of the soil.

The fundamental equation of ground-water flow can be derived from Darcy's Law

$$q = Q/A = -K\nabla H \qquad (3\text{-}1a)$$

plus a continuity equation

$$S\,\partial H/\partial t = -\nabla \cdot q \qquad (3\text{-}2)$$

to yield

$$S\,\partial H/\partial t = \nabla \cdot K \nabla H \qquad (3\text{-}3)$$

where ∇ = del operator, or

$= \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$

S = storage coefficient

H = hydraulic head

K = hydraulic conductivity

Equation 3-3 can take many forms depending on whether the flow is steady state or transient and whether the media is homogeneous or heterogeneous and isotropic or anisotropic. Refer to the references at the beginning of the chapter for the various forms of the equation. Steady-state flow occurs when the magnitude and direction of the flow velocity are constant with time at any point in the flow field. Transient flow (unsteady flow) occurs when the magnitude or direction of the flow velocity changes with time at any point in the flow field.

Each form of the ground-water flow equation has an infinite number of solutions. To get a specific solution for a problem, the initial and boundary conditions must be specified. Initial conditions pertain to transient flow cases only, and specify the value of the dependent variable (head) initial time ($t = 0$). Boundary conditions are where the head or flux conditions at the boundaries of the problem must be specified as either prescribed head (Dirichlet) or flux (Neumann). For prescribed head conditions, the head is

specified at points along the boundary. For prescribed flux conditions, the flux of water (either in, out, or no flow) is specified at points along the boundary.

3.2. PRIMER ON CONTAMINANT TRANSPORT

This section is intended to provide a brief summary of the background information necessary to understand the transport of contaminants in ground water. The chapter begins with the basic equation for advective-dispersive transport and discusses the important terms in detail.

3.2.1. Advective Dispersion Equation

Movement of contaminants in the soil can be described by the following equation (van Genuchten and Alves, 1982)

$$\partial c/\partial t = D^* \partial c^2/\partial x^2 - V^* \partial c/\partial x - kc \qquad (3\text{-}4)$$

where C = solution concentration (mg/l)

$D^* = D/R$

$V^* = V/R$

R = 1 + (B/N) Kd = retardation factor (dimensionless)

D = dispersion coefficient (cm^2/day)

V = average interstitial pore-water velocity (cm/day)

k = degradation rate coefficient (day^{-1})

B = bulk density (g/cm^3)

N = effective porosity (dimensionless)

Kd = partition coefficient (ml/g)

Equation 3-4 states that the change in contaminant concentration with time at any distance, (X) is equal to the algebraic sum of the dispersive transport (1st term to right of equal sign), the convective transport (2nd term), and the degradation or decay of the compound (3rd term). Van Genuchten and Alves (1982)

note that various modified forms of this same basic equation have been used for a wide range of contaminant transport problems in soil science, chemical and environmental engineering, and water resources.

Equation 3-4 considers only one-dimensional transport of contaminants. This equation considers dispersion, advection, equilibrium adsorption (linear isotherm), and degradation/decay (first-order kinetics).

A wide variety of physical processes occur in ground-water systems which are important, to varying degrees, in the analysis of contaminant fate and transport. A more detailed description of these processes is given by Fischer et al. (1979) and Schnoor (1985). Some of the important hydrologic transport processes include:

- Advection -- The process by which solutes are transported by the bulk motion of the flowing ground water. As a result of advection, nonreactive contaminants are carried at an average rate equal to the average linear velocity of the water.
- Molecular Diffusion -- The process whereby ionic or molecular constituents move under the influence of their kinetic activity in the direction of their concentration gradient. Diffusion occurs in the absence of any bulk hydraulic movement of the solution. Diffusion is a dispersion process which is important only at low velocities.
- Hydrodynamic Dispersion -- The tendency of a contaminant to spread out from the path that it would be expected to follow according to the advective hydraulics of the flow system. Dispersion occurs because of mechanical mixing during fluid advection and because of molecular diffusion due to the thermal-kinetic energy of the solute particles.

- Mechanical (Hydraulic) Dispersion -- Dispersion that is caused entirely by the motion of the fluid.
- Longitudinal Dispersion -- Spreading of the contaminant in the direction of bulk flow.
- Transverse Dispersion -- Spreading of the contaminant in the directions perpendicular to the bulk flow.

Most contaminant transport models simulate hydrodynamic dispersion only and disregard the molecular diffusion component because it is so small. Some models do simulate the molecular diffusion component for cases where the ground-water velocity is small and the diffusive component can become significant.

Most models available today simulate contaminant transport using a form of the advective-dispersion equation. Increasing evidence suggests that the conventional advective-dispersive equation does not always adequately describe contaminant transport in a natural geohydrologic system as a result of 1) random variations in ground-water velocity that are induced by media heterogeneities, and 2) the failure of Fick's diffusion law to properly describe hydrodynamic dispersion at field scales (Gelhar et al., 1979; Gelhar and Axness, 1983; Smith and Schwartz, 1980; Matheron and DeMarsily, 1980; Dagan and Bresler, 1979; and Dagan, 1982). Field determinations of dispersivity have shown a scale dependence, that is, the observed dispersivity was dependent on the size of the experiment rather than being exclusively a media property. A more detailed discussion of recent findings regarding dispersivity can be found in Gelhar and Axness (1983), Freyberg (1986), Gelhar et al. (1985), and Pickens and Grisak (1981).

3.2.2. Attenuation and Degradation Mechanisms

The primary physical processes included in contaminant transport models are sorption and degradation. The kinetic formation and rate constants used to describe these processes are typically based on laboratory measurements. The results of the laboratory measurements are incorporated in the models as source or sink terms in the general advection dispersion equation.

The direct transfer of controlled experimental results to natural ground-water systems is not always straightforward. Uncertainties arise in the definition of driving forces such as whether the system is aerobic or anaerobic, the pH of the natural system, and the chemical equilibria of the natural system (i.e., whether other ions are present which may catalyze or retard various reactions and the organic content of the soil). One of the biggest problems with simulating natural ground-water conditions in the laboratory is properly representing the geologic media (i.e., layering, heterogeneity, hydraulic conductivity, porosity, etc.). In spite of the uncertainties, these processes are incorporated in many ground-water models, and some models have been calibrated to field conditions. Careful calibration has shown that they are useful for representing the transport of various chemicals.

Most of the available models use some form of first-order reaction kinetics to represent the different processes that will degrade or transform a specific chemical. For a simple first-order reaction, ignoring all other mechanisms, the concentration can be represented as a first-order differential equation

$$dc/dt = -kc \qquad (3\text{-}5)$$

where k is the rate constant (1/T). In the simpler models, the rate constant does not change, in the more complex models the rate constant(s) may be variable

and calculated as a function of changing environmental conditions. The analytical solution to this equation when k is a constant is

$$C(t) = C_0 e^{-kt} \quad (3\text{-}6)$$

where Co is the initial concentration. From this equation an estimate of the time required for the process to reduce the contaminant concentration below a fixed "action level" can be determined.

$$t = \frac{\text{Ln } C(t)/C_0}{-k} \quad (3\text{-}7)$$

Often the reaction rate of various chemicals subject to different kinetic processes are characterized in terms of their half life, $t_{1/2}$. This is a measure of the time required for some kinetic process to degrade or transform the specific chemical to one-half of the initial concentration. The half-life is calculated from Equation 3-7 with the $C(t)/C_0$ set to 1/2.

A brief description of the sorption and degradation processes is included for potential users unfamiliar with the terminology. Much more detailed descriptions including assumptions, limitations, kinetic formulations, and methods for estimating rate constants are given by Bohn et al. (1979), Bolt and Bruggenwert (1978), Peterson et al. (1986), and Freeze and Cherry (1979).

3.2.2.1. Sorption -- Sorption is a transfer process whereby dissolved chemicals in the ground water become attached to sedimentary materials and/or organic matter. The process is commonly described using a partition coefficient. The definition of the partition coefficient is the ratio of the mass of chemical sorbed on the solid phase divided by the mass of chemical left in solution at equilibrium, as shown in Equation 3-4. The important assumptions in using this formulation are: 1) the chemical is at trace concentrations, hence the sorption isotherm may be assumed to be linear; and 2) the system is at equilibrium.

Some problems associated with field application of this concept include: 1) many chemicals exhibit nonreversible sorption characteristics, hence, desorption from sediments to the water column may not be correctly represented; 2) sorption characteristics are dependent on particle size (sand, silt, clay) and particle size is variable in a natural system; 3) sorption characteristics are dependent on pH and ionic strength which are often variable in a natural system; and 4) the presence of other compounds in a natural system results in competition for sorption sites on the soil matrix. Some of the compounds that may be strongly affected by sorption include heavy metals and many organic compounds. For organ compounds, partition coefficients are frequently normalized to the organic carbon content of the soil (Karickhoff, 1980, 1981, and 1984; and Gschwend and Wu, 1985). As noted previously, the relationship between dissolved and adsorbed forms of a contaminant is usually represented in the form of an equilibrium partition coefficient (Kd). The partition coefficient is defined as the ratio of the mass of the substance adsorbed to the particulates (per unit mass of particulates) over the dissolved concentration of the solute. The retardation factor is calculated from the partition coefficient, bulk density, and the effective porosity, and is a number which describes how many times slower than water a contaminant travels through a porous media system.

3.2.2.2. Degradation -- Degradation in ground water systems may result from one or more of three mechanisms: biological transformations, hydrolysis, or chemical reactions. Biological transformations are reactions due to the metabolic activity of aquatic microbes, primarily bacteria. Depending on the specific chemical, the transformations may be very fast due to the presence of enzymes and for other compounds the process may be very slow. The rate and

nature of by-products will also be dependent on the availability of oxygen. In unsaturated aerated zones, aerobic degradation will predominate, while anaerobic mechanisms will be controlling in anoxic zones. For chemicals where the transformation is fast, degradation is often the most important transformation process in the aquatic environment. Various kinetic formulations have been proposed including first- and second-order forms. The rate coefficients are known to be a function of temperature, pH, and available nutrients. The second-order kinetic formulations describe the degradation rate as a function of the concentration of the compound and the bacterial population which is changing as the compound is degraded. A variety of organic compounds may be subject to degradation. A discussion of various compounds is provided by Klecka (1985).

Hydrolysis is the reaction of chemicals with water. Typically a compound is altered in a hydrolysis reaction by the replacement of some chemical group of the compound with a hydroxyl group. The hydrolysis reactions are commonly catalyzed by the presence of hydrogen or hydroxide ions and hence the reaction rate is strongly dependent on the pH of the system. Hydrolysis reactions alter the structure of the reacting compound and may change its properties. The new compound is usually less toxic than the original compound, but this is not always the case depending on the specific reaction. Neely (1985) lists several functional groups that are susceptible to hydrolysis reactions including alkyl halides, amines, carbamates, carboxylic acid esters, epoxides, lactones, phosphoric acid esters, and sulfonic acid esters. For many functional groups, and therefore a considerable number of compounds, hydrolysis will not occur.

Chemical reactions refer to the interaction of contaminants with other chemicals in the ground water besides the water itself. Many chemical reactions

are of the oxidation-reduction type (redox). Redox reactions involve the transfer of electrons from one chemical (the reducing agent) to the other (the oxidizing agent). In the process, toxicity and solubility properties are often changed. Possible couples for redox reactions can be determined from oxidation potential tables.

3.2.3. Definition of Terms

Throughout this report a number of terms or phrases are used which may be interpreted as having somewhat different meanings by different readers with various backgrounds, experience, and general inclinations. In an attempt to avoid any misinterpretations, this section defines the specific meaning intended for a few key terms.

1. Calibration -- In this document we will use the term calibration to describe the initial phase of a modeling study where the input coefficients of a model are adjusted in an attempt to match measured field data (e.g., velocity, concentration). The types of coefficients that are commonly adjusted in a ground-water flow model are recharge and discharge, hydraulic conductivity or transmissivity, and porosity. The types of coefficients that are commonly adjusted in a transport model include dispersion coefficients, degradation rate constants, sorption properties, and possibly source and sink terms.
2. Validation -- The term validation will be used to describe a separate step of a modeling study where the calibrated model (i.e., fixed coefficients, no more adjustments) is applied to a different set of conditions and the results are compared with a separate set of field data. The validation phase is an attempt to see if the model can reproduce field data under conditions different than those used in the calibration phase. This

distinction between calibration and validation is easy to define and appropriate from an idealistic point of view. Real applications may find it impossible to obtain a separate data set or the validation phase may indicate poor model performance and the validation data set might be used for additional calibration. Under these circumstances, larger uncertainty in the model results, and this needs to be incorporated into any decision-making process.

3. Verification -- The term verification will be used to define the process of comparing the results of one model against those of another model. For example, it is common to compare the results of a tested and accepted analytical solution/model against a more sophisticated numerical model in order to verify the numerical solution technique.

4. Mathematical Model -- The term mathematical model will be used to describe the mathematical representation of the physical system. The model may represent an analytical solution to these equations and in other cases the model may be an approximate numerical representation of these equations. In some cases, the models based on analytical solutions are simple enough that the calculations can be performed using a hand calculator. In other cases the analytical models are more complex and often are implemented as a program to be run on a computer. All of the numerical models are implemented as programs to be run on a computer. Computer models are often referred to as codes or computer codes. We have used the term model, as opposed to code, wherever appropriate in this document. Mathematical model in this definition is equivalent to mathematical systems model involving multi-processes.

5. Process Equation -- The mathematical representation of a physical phenomenon or process for a system. For example, solute transport in a saturated system may be described by the solution of the advective dispersion equation. A process equation in this definition is equivalent to a multi-process equation involving several different phenomena.
6. Analytical Models -- A computer program written to solve a particular process equation. For example, the AT123D model (Yeh, 1981) is a computer program written to analytically solve the advective dispersion transport equation for a variety of simple initial and boundary conditions.
7. Numerical Model -- A computer program written to solve a particular process equation for which no general solution exists. For example, the CFEST model (Gupta et al., 1986) is a computer program, part of which is written to numerically solve the advective dispersion transport equation for a variety of simple or complex initial and boundary conditions.

The relationship between the above terms may be thought of as follows. A mathematical model consists of two aspects: a process equation and a solution technique to solve the process equation. An analytical solution solves a very simple process equation analytically by hand calculations. An analytical model solves a more complex, but still relatively simple, process equation analytically with a computer program. A numerical model solves a simple or complex process equation numerically with a computer program. In the context of this document, mathematical model refers to all three solution techniques (analytical solution, analytical model, numerical model) of a process equation. The more detailed the specific application, the more complex the process equation. The complexity of the process equation dictates the solution technique required.

The term analytical or numerical code typically refers to the computer program (the set of computer instructions written in a programming language and acted on by a computer), whereas an analytical or numerical model is the implementation of the code with a specific data set (either site specific or generic) to test the simulated representation of the system against observed or measured behavior. In this document the analytical solutions referenced in Table 5-1 and the analytical and numerical codes summarized in Appendix A are all included in the general category of mathematical models.

8. Objectives Criteria -- Criteria related to the level of modeling detail required to meet the objectives of the study. In the context of model selection, objectives are classified into two categories: perform a screening or generic study where simple analytical solutions/models would most likely be used, or perform a detailed study using numerical models.
9. Technical Criteria -- Criteria related to a code's ability to simulate the transport and fate phenomena of importance. These criteria are based on the physical, chemical, and biological characteristics of the site and the contaminant of interest.
10. Implementation Criteria -- Criteria related to the ease with which a code can be obtained and its acceptability demonstrated. Relevant factors include sources of the code, documentation, verification, and validation.
11. Screening and Detailed Assessment -- The types of modeling analysis that are described in this document may be very broadly categorized as screening or detailed (site specific) exposure assessment studies. Obviously, these categories cannot be distinguished by definitive criteria but rather there is more of a "gray" area between the two. We have chosen to use the term screening analysis to represent studies where limited calibration and

validation data are available and the uncertainty associated with the predicted results is comparatively large, somewhere in the nature of an order of magnitude. The term detailed or site-specific analysis is used to represent studies where a smaller uncertainty in the predicted results is necessary, on the order of a factor of two to ten. Calibration and validation data are necessary in order to reduce the uncertainty inherent in the results and also attempt to quantify the bounds associated with the uncertainty through the validation phase and sensitivity studies. The models used for a screening analysis are generally easier to use but make certain restrictive assumptions. The more complex site-specific assessment models are more difficult to use and generally do not make as many restrictive assumptions; the input data requirements, however, may be substantially greater.

4. GENERAL GUIDELINES AND PRINCIPLES OF MODEL SELECTION CRITERIA

This chapter discusses some of the general guidelines and principles related to model selection criteria. The first section discusses the steps that should be taken in the overall modeling process. The second section provides a general discussion of the model selection process and discusses the three principle criteria used to select a model: objectives criteria, technical criteria, and implementation criteria. The last three sections discuss some important issues related to model selection: model selection vs model application familiarity with a model, and model reliability.

4.1. OVERVIEW: MODELING PROCESS

The selection of models for the analysis of exposure to contaminants involves factors addressing a number of issues, not all of which are amenable to expression in specific criteria. Certain judgmental factors are better suited to statement in the form of general guidelines and principles. Many of these arise from the nature of the overall modeling process of which model selection is but a single step. Five general steps may be identified in the modeling process. Although model selection is meant to be the primary emphasis of this report, the different steps influence each other and need to be described. The five general steps are:

1. Problem Characterization -- The analyst clearly identifies the exposure assessment study objectives and constraints.
2. Site Characterization -- The analyst reviews available data on the site, develops a conceptual model identifying processes of interest, performs a screening analysis; if a modeling study is necessary, the analyst then identifies data needs and fill those needs. The results of the site

characterization will determine technical specifications for model selection by identifying the single processes at the site.

3. Model Selection Criteria -- The analyst matches the objective, technical, and implementation criteria to available models and selects the most appropriate model(s).
4. Code Installation -- If the model selected is a computer code, the code is installed on the computer system and tested to document proper installation and ability to reproduce accepted solutions to standard problems.
5. Model Application -- The verified model uses site characterization data as input for the exposure assessment simulation.

These five general steps are not the model selection criteria but rather the overall process by which a problem is identified and a model selected to perform an exposure assessment study. Model selection criteria is listed as the third step in this process. The two previous steps, problem characterization and site characterization, are crucial in the selection of an appropriate model(s). While the steps can be considered sequential in nature, it is important to recognize interactions and feedback mechanisms between them. For instance, knowledge of the model selection criteria is important to assure that site characterization is adequate and properly formatted. An understanding of code installation procedures is required for proper scheduling and resource allocation. Familiarity of candidate models is needed to assure that site characterization provides necessary input data.

Problem characterization is important because a wide variety of models and modeling approaches are available. Different modeling techniques are suitable for different objectives and physical problems. The exposure assessment objective must define what the goal of the analysis should be and must also be

defined in a manner consistent with known project constraints such as schedule, budget, and other resources.

Site characterization is an important step that needs more description because the conceptualization of the physical system, whether it is a specific site or a generic problem, will obviously influence any additional steps. If the objectives of the exposure assessment are to evaluate an existing contamination problem, then this step should include the availability of field measurements in the specific study area. Depending on the problem, the field measurements may include geologic structure data, pump tests, recharge/discharge data, elevations of surface water bodies, contaminant sampling, and source characterization. Field measurements may identify the extent of the contamination problem and whether or not the concentration levels are above some regulatory or dangerous level. In addition, if these initial studies identify a contamination problem and a modeling study is to be performed, then the field measurements will be used in the selection of an appropriate model and for model calibration.

Model selection criteria (the primary goal of this report) is entirely dependent on the first two steps. This step is covered in more detail in the rest of this chapter and in Chapter 4.0.

Code installation only applies when the model chosen in the third step is a computer code. When a code is first obtained and installed on a specific computer system, it is essential that the model be tested to verify that it is working correctly and can reproduce suitable example problems. Various computer systems and the necessary model software may have a variety of differences, some distinct and others more subtle. These differences may require modifications to an acquired code (e.g., double precision arithmetic or changing output formats)

on different computer systems. Verification assures that modifications have not changed model results significantly. This step should be performed by the person doing the actual model analysis.

Model application relates the use of a model in an attempt to answer the questions to the use of a model in an attempt to answer the questions defined in the objectives. Depending on the objectives of the analysis, this step may consist of several parts including calibration, validation, and application to evaluate different conditions or scenarios.

4.2. OVERVIEW: MODEL SELECTION CRITERIA

There are three factors which dictate the level of complexity of the mathematical model chosen in the selection process: 1) objectives criteria, 2) technical criteria, and 3) implementation criteria.

4.2.1. Objectives Criteria

The first level of consideration when selecting a mathematical model is related to the objectives of the study. Based on the objectives, the analyst can limit the choice to either simple analytical solutions/models or to more complex numerical models.

The objectives criteria refer to the level of modeling detail required to meet the objectives of the study. There are many different objectives of modeling studies, however, in the context of model selection, all objectives can be classified in two broad categories: 1) to perform a screening study or 2) to perform a detailed study.

A screening study is one where the purpose is to make a preliminary screening of a site or to make a general comparison between several sites. A

screening assessment can also be generic (i.e., not site specific) where the objective is to compare several hypothetical cases or designs.

A screening study may be appropriate when sufficient data is not available to properly characterize the site. Although lack of data is no excuse for not modeling a site correctly, often there are times when a screening comparison of cases/sites can be quite helpful in analyzing a problem. A screening study can help direct the data collection effort at a site. For generic studies, it is most often not possible to select a detailed data set which is representative of all the hypothetical sites/cases being simulated. By virtue of the fact that it is a generic study, the data base is typically quite simple such that it is representative of several sites/cases.

A detailed study, on the other hand, is used when the objective is to make a detailed assessment of the environmental impact, performance, or safety of a specific site. This type of study requires detailed data for a specific site or for a number of sites, and the results of the study are typically used to make specific decisions regarding the site or sites. For example, a detailed study might involve predicting concentration of a particular contaminant at a specific aquifer location. The results of the study would be used by decision makers to determine whether remedial action is needed at the site.

Screening and detailed studies usually require the use of screening and detailed models, respectively. A screening model would typically be an analytical solution or model with minimal data requirements. Usually these analytical solutions/models are used for special, simplified physical conditions that represent the behavior of particular physical processes when isolated from other effects. Compared to numerical models, screening models require less data, are easier to implement, and are less expensive to run.

Detailed models are typically numerical models which have more extensive data requirements, are more difficult to implement, and cost more to operate (take longer to set up, calibrate, and evaluate results and require more computer time) than analytical models/solutions. Detailed models usually have more realistic initial and boundary conditions and possibly more time-dependent inputs and outputs than screening models.

Based on the objectives of the study (screening or detailed), the analyst or modeler will select either a screening or a detailed model. The specific model to be used will be selected based on the technical selection criteria discussed below.

4.2.2. Technical Criteria

The second level of consideration when selecting a mathematical model is the technical criteria. Technical criteria are those criteria related to the mathematical model's ability to simulate the site-specific contaminant transport and fate phenomena of importance. These criteria are based on the physical, chemical, and biological characteristics of the site and the contaminant of interest. The characteristics of the site and the processes that need to be simulated are determined from the hydrogeologic and contaminant data and the conceptual model of the site.

With regard to model selection, the technical criteria can be divided into three categories: 1) transport and transformation processes, 2) domain configuration, and 3) fluid(s) and media properties.

4.2.2.1. Transport and Transformation Processes -- Transport and transformation process criteria relate to those significant processes or phenomena known to occur on site that must be modeled in order to properly represent the site. The transport process is the physical migration process controlled by adsorption,

attenuation, diffusion, dispersion, volatilization, and density effects related to temperature and/or concentration. The transformation processes that effect contaminant migration can be divided into chemical and biological processes. Chemical processes include complexation, hydrolysis, chemical degradation, and oxidation-reduction. Biological processes include biodegradation, biological transformation, metabolism, and respiration. The mathematical model selected must be able to simulate all the relevant physical processes occurring within the specified environmental setting.

4.2.2.2. Domain Configuration -- The second category of the technical criteria relates to the ability of the model to represent the domain configuration of the geohydrologic system. The relevant parameters related to geometry include:

- Water table or confined flow system
- Porous media or fracture flow
- Steady-state or transient flow
- Single- or multi-phase flow
- Constant, flux, or no-flow boundary conditions
- Single- or multi-layer system
- Constant or variable thickness layers
- One-, two-, or three-dimensional system
- Source configuration
  - Constituents
  - Point, line, or area source
  - Initial value, constant, or variable source

When high levels of resolution are required to predict contaminant concentrations for comparison to health or design standards, it is generally necessary to simulate site-specific geometry and dimensionality for which

numerical models are most appropriate. If simplifying the site geometry can be defended on a geotechnical basis, then the use of a simpler analytical model/solution may be justified.

Analogously, the natural dimension of the system can be reduced if at least one dimension can be integrated to a single value. For example, if a contaminant is distributed evenly in a single aquifer in the vertical direction, the level of contamination can be expressed as a single value in a two-dimensional transport model of the horizontal plane (x-y). In effect, the contaminant mass in the vertical (z) dimension is integrated into a single representative value.

4.2.2.3. Fluid(s) and Media Properties -- The third category of technical criteria corresponds to the ability of the mathematical model to represent the spatial variability of fluid(s) and media properties of the geohydrologic site. The relevant issue in this category is whether the site can be considered homogeneous or heterogeneous with regard to hydraulic conductivity, recharge, porosity, and specific storage. If homogeneous conditions can be assumed, it is often possible to simulate the site with an analytical solution/model. Heterogeneous conditions almost always require a numerical model. For example, an aquifer may consist of several geologic material types all having different hydraulic conductivities. Proper simulation of the spatially variable hydraulic conductivity would require the use of a numerical model.

As stated above, the objectives criteria will direct the analyst to select either a screening or a detailed model. Once the level of model has been decided, the technical criteria will direct the analyst to the specific type of model needed to properly simulate the transport and transformation aspects of the environmental setting.

4.2.3. Implementation Criteria

The third level of consideration when selecting a mathematical model is related to the implementation criteria. Implementation criteria are those criteria dependent on the ease with which a model can be obtained and its acceptability demonstrated. Whereas the technical criteria identify models capable of simulating the relevant phenomena within the specified environmental setting, the implementation criteria identify documentation, verification, validation requirements, and ease of use so that the model selected provides accurate, meaningful results.

Relevant questions to be considered concerning the implementation of a particular model include: 1) what is the source of the model and how easy is it to obtain (i.e., is it a proprietary model); 2) are documentation and user's manuals available for the model and, if so, are they well written and easy to use; 3) has the model been verified against analytical solutions and other models and, if so, are the test cases available so the analyst can test the model on his computer system; and 5) has the model been validated against field data?

The technical criteria can be used to narrow the model selection to a few codes in the same general category. The implementation criteria can then be used to further narrow the decision to one or several of the technically acceptable models.

4.2.4. Other Factors Affecting Model Selection

Other general factors related to model selection which should never override the technical or implementation criteria include data availability, schedule, budget, staff and equipment resources, and level of complexity of system(s) under study. Schedule and budget constraints refer to the amount of

time and money available for the assessment. If both analytical and numerical models meet the selection criteria, time and cost may be considered factors for electing to use an analytical approach. Analytical solutions/models are easier to install on a computer system, are more quickly mastered, and are dependent on more easily-obtainable input data than numerical models. The time factor will be of increased importance if staff are not familiar with any of the appropriate models. In this case, schedule considerations may dictate selection of a different modeling team; one experienced with the appropriate models.

Staff resources are also a major consideration in modeling. Regardless of the quality of the model selected, the expertise of the analyst has a major impact on model results. This can also impact model selection when the analyst is familiar with one or more of the appropriate models. In the simplest case, if the analyst has direct experience with an acceptable model, then that model is preferred. Similarly, if the analyst has experience with a specific type of model (e.g., finite element vs finite difference), one of that type should be selected. In certain cases, familiarity with a model more complex than required may dictate use of that model rather than a simpler one since there will be no loss of resolution and the added staff experience would compensate for time and cost differences. In no case, however, should familiarity with a model dictate its selection when it does not satisfy the technical and implementation criteria. In practice, many models are rightfully applied to situations which are not fully compatible with the model's design characteristics. However, justification of the choice should indicate the correctness of the model's use.

Hardware requirements are similar to staff requirements. The more complex mathematical models require more powerful computers with larger mass storage

devices and extra peripheral equipment. If both analytical and numerical models meet the selection criteria, available hardware may dictate the use of the simpler analytical models. If a sophisticated model is required and adequate equipment is not available, alternate means of conducting the modeling must be found. Equipment constraints cannot be used to select a model other than those meeting the selection criteria.

As noted in the preceding paragraphs, subjective factors such as objectives, schedule, budget, and staff and equipment may be used to select one model from a group of models all found to meet selection criteria. Alternately, subjective factors may dictate use of a different modeling team to improve the quality of results obtained from a given model. Under no circumstances, however, shall subjective factors be used to select a model which otherwise fails the selection criteria.

In summary, the first step of the model selection process is to define the objectives of the study. If the objective is to perform a screening-level or generic type study, a simple analytical solution/model or a simple numerical model should be selected. If the objective is to perform a detail-level study, a more complex numerical model should be selected unless the study area is such that it can be simulated on a technically sound basis with a simpler model.

The decision as to which category of models or type of model can accurately simulate a site or perform an assessment is based on the technical criteria. The technical criteria are based on a model's ability to correctly simulate the transport and transformation processes, domain configuration, and fluids and media properties of a site. Depending on the objective of the study, the technical criteria can be used to narrow the selection of either screening or detailed models.

Once the appropriate models have been selected on the basis of technical criteria, the list can be further narrowed by use of the implementation criteria. The implementation criteria relate to factors such as availability of models, documentation, verification, and validation.

If a list of models still remain after satisfying the objectives, technical, and implementation criteria, the final decision should be based on such subjective factors as schedule, budget, and staff and equipment resources. Under no circumstances, however, should subjective factors be used to select a model which otherwise fails the selection criteria.

4.3. MODEL SELECTION VS MODEL APPLICATION

While this document is concerned with the issue of model selection, it is important to realize that in most cases the biggest differences in model predictions are a result of how the model is applied, not which model was selected. For most modeling studies, there are typically a number of models which satisfy the objectives, technical, and implementation criteria. If all of these models are applied to the same data set, they will all obtain virtually the same results. Differences may arise based on how the initial and boundary conditions and grid (numerical models) are specified in the model, but in all cases these differences should be insignificant.

The big difference in modeling assessments results from how the model is applied, not from which model is selected. The difference in how the model is applied stems from the fact that different modelers interpret the same data set differently. For example, if you gave ten different modelers the same raw data set and the same model code, they would probably develop ten different models of the site based on ten different interpretations of the data. The differences in the models might be small in many cases, but it is not unreasonable that large

differences (i.e., completely different ground-water flow directions or contaminant concentrations) could occur; especially for large, complex data sets requiring a detailed modeling approach. If, on the other hand, you gave ten different modelers the same model input data set (i.e., the inputs are defined for them, not a raw data set) and ten different models, with which they were very familiar, they should all arrive at about the same results.

Where the major differences occur in any modeling study is in the interpretation of the raw data and in the conceptualization of the study area. Since it is impossible to know everything about a ground-water flow/contaminant transport system, raw data are always subject to different interpretation. As a result of this basic fact, it is important to remember that the major differences in modeling studies will probably result from differences in the application of the model(s), not from the selection of the specific model to use.

4.4. FAMILIARITY WITH A MODEL

It is important to emphasize the importance of familiarity with a model, especially with regard to the more complex models. Detailed models, especially numerical models, can be quite complex with a large number of input variables, switches, outputs, and simulation/computer related requirements. Often it requires months or even years of experience and several studies to fully comprehend all the aspects of a model. Because of this, it is strongly advised that an analyst select a model with which he/she is familiar if it possesses all the selection criteria.

Many people feel that a more complex model should not be selected if a simpler model can do the job. They argue that the complex model requires too much data, will take longer to implement, and will cost more to run on the

computer than the simpler model. This may not be the case at all. Most complex codes can be run in a less complex mode which requires less data and implementation time. Even if computer costs are a little higher, the costs are almost always far offset by the savings in labor costs because the analyst is familiar with the model and can use it far more efficiently.

When dealing with the more sophisticated numerical models, only analysts familiar with the selected model should perform the assessment. If experienced persons are not available within the group, expert help from outside the group should be obtained. Simpler models can be used by analysts with little or no specific experience with the model. However, the work should be reviewed by a more experienced user to ensure that the model was set up and the results were interpreted correctly.

4.5. MODEL RELIABILITY

Because a natural ground-water system is very complex and heterogeneous, a model will never form an exact replica of the system. Because every model will inevitably be a simplification of the actual system, mathematical models should not be used to make "exact" predictions of ground-water flow or contaminant concentrations. Ideally, models should only be used to make comparisons between cases, whether site specific or generic.

When developing a model of a study area, simplifications must be made at every step in the process. The simplifications are a consequence of limitations in the acquisition of field data, limitations in developing a conceptual model of the systems, limitations in properly representing the data and physical processes in the model, and limitations in predictive mathematical theory for some physical processes. Because of all the limitations and simplifications, it is often difficult to place a great deal of confidence in predictive model

results (i.e., prediction of a contaminant concentration at a well). When comparing various cases or scenarios with a model, however, all the cases are subject to the same limitations and simplifications. Therefore, model results are more reliable in a situation where one case or alternative is compared to another.

Another method by which model results can be made more useful is to perform a sensitivity analysis. A sensitivity analysis is an analysis that quantifies the change in a specific performance assessment measure (i.e., ground-water velocity or concentration) resulting from a change in a specific input parameter or set of parameters to the model. For example, the model could be used to predict a range of ground-water velocities based on a range of hydraulic conductivities and gradients thought to be representative of the aquifer. A sensitivity analysis is a means of dealing with the inherent uncertainty which exists in the measurement of many hydrogeologic and contaminant transport parameters.

Although the many limitations and simplifications make it difficult to place a lot of confidence in model predictions, the use of models to make such predictions can often be justified in that, in most cases, a model is the only means or the best means available to make the prediction. For sites with complex hydrogeologic conditions, the use of a model is often the only means of integrating all the data into a meaningful package. In all cases, no matter how simple the site or how extensive the input data, model output or predictions always need careful evaluation because they are generally only as accurate as the model input data and the knowledge of the system upon which the model is based. Model results, whether "exact" predictions, a comparative analysis or a sensitivity run should always be considered as a guide to the probable system

response. Despite their limitations, when properly applied, models are often the best tools available for assistance in making decisions on ground-water flow and contaminant transport problems.

5. MODEL SELECTION DECISION PROCESS

This chapter discusses the technical criteria used to select the appropriate mathematical model for a specific application. The first section provides a detailed discussion of the technical criteria and the errors associated with selecting one option over another. The second section briefly discusses the model selection process from the point of view of a reviewer from a regulatory agency. The last section groups the available models into categories and provides the framework for selecting the appropriate model or category of models based on the response to the technical criteria.

5.1. TECHNICAL CRITERIA USED FOR MODEL SELECTION

The technical criteria used to select the appropriate performance assessment mathematical model(s) for ground-water applications are outlined in Figure 5-1.

The first task in any contaminant transport analysis is to simulate the ground-water flow. The ground-water flow can be simulated separately from the contaminant transport, or both can be simulated with one model. However, each approach requires sequential simulations; first the ground-water flow followed by the contaminant transport. For this reason, Figure 5-1 is divided into two sections. The first section addresses the technical decisions that need to be made to select the appropriate ground-water flow model (or flow portion of a combined ground-water flow and contaminant transport model), while the second section addresses the technical decisions that need to be made to select the appropriate contaminant transport model.

The decisions that need to be made when selecting a ground-water flow/contaminant transport model are discussed in detail below. Guidance is

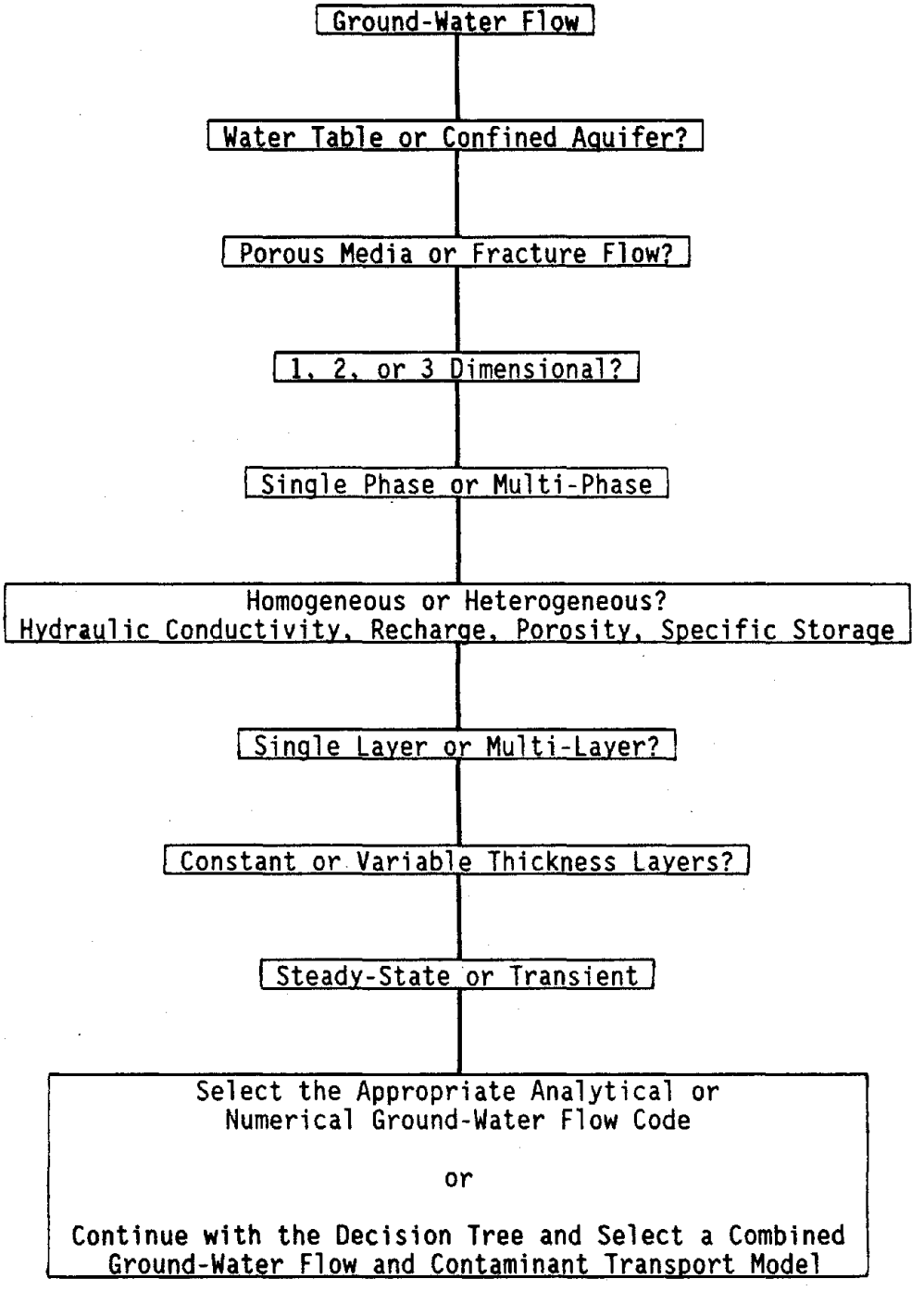

Figure 5-1. Code selection decision tree.

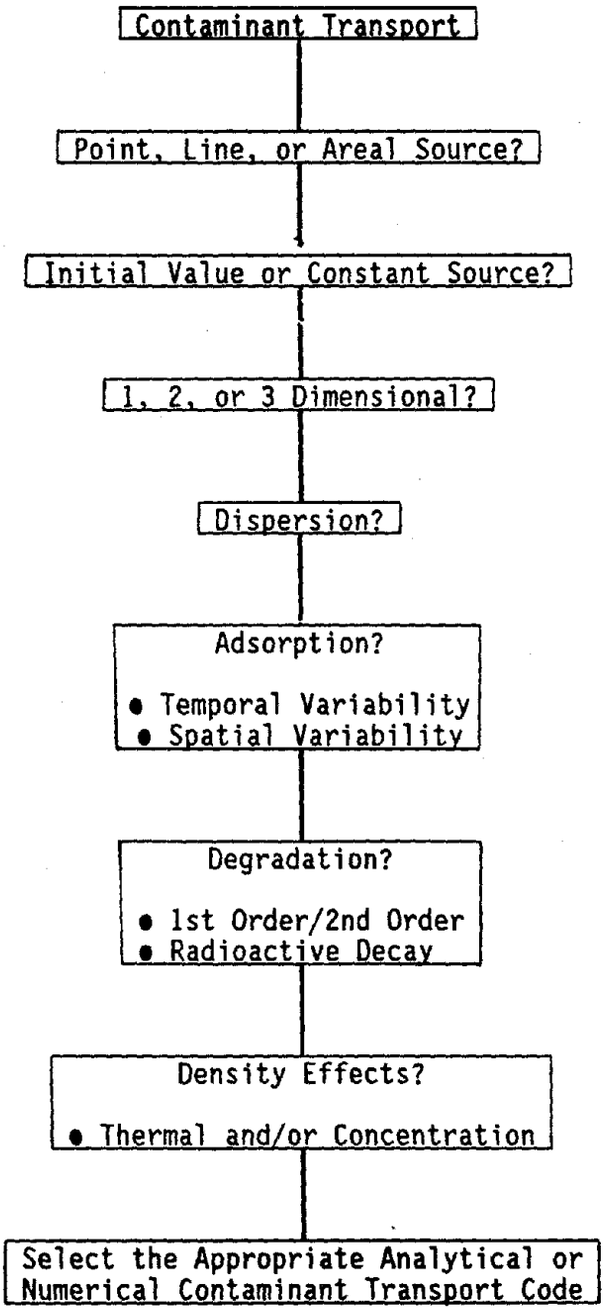

Figure 5-1. (continued)

provided for making each decision and some discussion is provided regarding the errors associated with making an incorrect choice (i.e., selecting a model that does not contain the desired feature); for example, the use of a porous media model to simulate fracture flow.

In all cases, the impact of an incorrect decision or the use of an incorrect feature of a model is difficult to quantify. For many cases, the errors are difficult to quantify because they are site specific; they depend on the actual site data. For example, the error associated with using a homogeneous hydraulic conductivity distribution where a heterogeneous distribution should have been used can only be quantified on a site-by-site basis. In other cases, the errors are difficult to quantify even for a site-specific application because the necessary parameters are unknown or cannot be measured. An example where it is difficult to quantify the associated error would be using a model that uses a uniform value of recharge over a study area versus one that uses a recharge distribution because recharge is difficult to measure in the field.

Many of the decisions that need to be made when selecting an appropriate model can be made on the basis of past experience. Although this document provides insight regarding decisions based on experience, there is really only one way to gain the knowledge that comes from experience and that is to get involved in modeling studies and in the selection of the appropriate models for those studies.

Several questions need to be answered when selecting an appropriate groundwater flow model. Such questions deal primarily with the flow media, but some questions address such aspects as steady-state or transient flow and whether the fluid is single or multi-phase. The following paragraphs list the questions

needing to be answered when selecting an appropriate flow model with a brief explanation of each.

1. Are you simulating a water table (i.e., unconfined) or a confined aquifer, or a combination of both (i.e., conditions change spatially)?

   The analyst needs to select a model which can simulate the type of aquifer conditions which exist at the site, either water table, confined, or a spatial combination of both. Most ground-water flow models simulate confined aquifer conditions, whereas not all models can simulate water table conditions or a combination of both. The reason for this is that the solution for the water table case is more complicated and requires more time to solve. As a result, it is not uncommon that a confined model will be used to solve a problem with water table or mixed water table and confined conditions.

   The problem associated with using a confined model for unconfined aquifer conditions is that the aquifer thickness is not allowed to vary. As a result, the transmissivity (defined as the aquifer thickness times the hydraulic conductivity) remains constant when it should be adjusting with the fluctuations in the water table. The error associated with using a confined model for unconfined aquifer conditions is small as long as the fluctuations in the water table are small compared to the total thickness of the aquifer. Small fluctuations are usually defined as where the water table elevation changes by less than 10% of the total aquifer thickness. This criterion is valid under most circumstances. Typically, the criterion

is violated when there are large stresses on the system such as pumping or recharge, or when the aquifer is very thin (in general, less than 25-ft thick).

2. Is the ground-water flow through porous media, fractures, or a combination of both?

The analyst needs to select a model which can simulate the types of media which exist at the site, either porous media, fractured media, or a combination of both. Most ground-water flow models simulate porous media. Although few models are designed to simulate fracture flow, most numerical models can handle soils with different porosity (i.e., dual porosity). As a result, to date most fracture flow systems are approximated by porous media models. The validity of this assumption is dependent on two factors: 1) how highly fractured are the media, and 2) what is the scale (size) of the fracture system. In this approximation, it is generally assumed that a highly fractured system can be thought of as a rock that is so highly fractured that it resembles a continuum porous medium. A quantitative definition of a highly fractured system does not exist. However, for this approximation, highly fractured could possibly be considered as fractured rock with an effective porosity resembling the effective porosity of a porous media which is typically on the order of 10 to 25%.

The ability to simulate a fractured system with a porous media model is also scale dependent. The larger the scale of a fractured system, the more the flow pattern through fractures represents flow in porous media. As the

scale gets smaller and smaller, it eventually gets down to simulating the flow in a single fracture which cannot be simulated with a porous media model.

In some instances, a finite-element model can be used to simulate flow in faults, where a fault is defined as a large fracture. The fault can have a higher or lower permeability than the surrounding rock depending on the nature of the rubble in the fault zone. In this case, the fault is simulated as a series of long, narrow elements in the model and the hydrologic properties (hydraulic conductivity, porosity, etc.) of those elements are set accordingly.

3. Is it necessary to simulate three-dimensional flow or can the dimensionality be reduced without losing a significant amount of accuracy?

The analyst needs to select a model which can simulate the dimensionality needed to properly represent the site, either one-, two-, or three-dimensional.

In general, models should be selected in three dimensions unless it can be shown that the degree of media homogeneity and spatial symmetry of the aquifer are such that they justify the selection of a lower dimensional model. If, for example, the problem consists of a single aquifer with uniform hydraulic properties and concentrations in the vertical (z) dimension, then a two-dimensional x-y simulation is justified. If the hydraulic properties and concentrations are also uniform in one of the two

horizontal dimensions (x or y in addition to z), then one is justified in making a one-dimensional simulation.

Lower dimensional simulations are not always made because they are justified based on the homogeneity or spatial symmetry of the data. In many instances, a lower dimensional simulation is made because the data are not available to perform a three- or two-dimensional simulation, or even to know if the higher dimensional simulation is required. The use of a three-dimensional model without adequately detailed site characterization data can easily lead to incorrect results.

Even though a lower dimensional simulation is performed where a higher level model was warranted, the results can still be quite useful in assessing a particular problem. The lower dimensional model can be used as a screening-level model to make numerous, low-cost runs which, in many cases, can provide valuable insight into a problem.

It is important to remember that performing a complete three-dimensional analysis does not eliminate uncertainty in the results. It is virtually impossible to completely characterize a ground-water flow/contaminant transport system, and no matter how well the system is characterized, the model, whether one-, two-, or three-dimensional, is always a simplified representation of the real system. Three-dimensional model results, as well as one- and two-dimensional model results, need to be analyzed very carefully to determine if they make sense.

The dimensions of the ground-water flow model can be dictated by the needs of the contaminant transport model. For example, if the flow is occurring in a single homogeneous aquifer of constant thickness, a two-dimensional x-y model should be selected. However, if the contaminant plume is not uniformly distributed over the thickness of the aquifer or if a remedial action requires pumping from a screened interval less than the total aquifer thickness, then a three-dimensional transport model is required. If a three-dimensional transport model is required, then the flow should be simulated in three dimensions. It is possible to simulate the ground-water flow with a one-dimensional model and then simulate the contaminant transport with a three-dimensional model, but in this case the transport simulation will not truly be a three-dimensional simulation since the flow vector is in only one direction.

4. Are you simulating a single-phase (i.e., water) or a multi-phase (i.e., water and an insoluble contaminant) flow system?

The analyst needs to select a model which can simulate the type of flow system which exists at the site, either single-phase or a multi-phase system.

Very few mathematical models are available today which can be practically applied to a multi-phase ground-water flow problem. Much of the original research in this area was performed in the petroleum industry for the analysis of three-phase flow of oil, gas, and water. The petroleum industry work has been adopted in the ground-water industry to study

multi-phase flow between water and contaminants, but the ground-water efforts are in the infant stages.

Most contaminant transport analyses assume the contaminant is soluble in water. This single-phase approach is accurate enough for almost all practical purposes. For the case where the contaminant is immiscible in water, the single-phase approach does not apply. If a single-phase model with proper boundary conditions such as an area source of continuous release is applied to a multi-phase problem, it can provide some insight into the extent of plume migration for a relatively large source of the immiscible contaminant phase which would float on the aquifer's surface or sink to the bottom of the aquifer. Significant inaccuracies are likely to arise if the contaminant travels with ground water along the flow line.

5. Can the system be simulated with uniform (homogeneous) or spatially variable (heterogeneous) values of hydraulic conductivity, porosity, recharge, and/or specific storage?

Homogeneous in this sense refers to spatially uniform values in the x direction or the x-y plane. Some mathematical models, particularly analytical solutions or simple numerical codes, only simulate a single value of a hydraulic property spatially. For example, the hydraulic conductivity or recharge may have to be uniform over the entire model region. In a heterogeneous model, on the other hand, many of the parameters (particularly the hydraulic conductivity and the recharge) can be specified on a node-by-node (finite difference) or an element-by-element (finite element) basis. Thus, it is possible to represent a spatial distribution of certain parameters over the study area.

Quantifying the errors associated with using a single average value versus using the actual distribution is difficult and very site specific. In a general sense, many of the criteria discussed above apply here. With regard to hydraulic conductivity, if all the spatial values are within a factor of 10, using a single average value is probably justified. If the spatial values of recharge, porosity, and storage do not vary by more than about 25%, using a single average value is probably justified. In most modeling studies, the recharge, porosity, and storage are not well enough known to define a spatial distribution. For site-specific, detailed studies, if spatially-variable values are required but are not available, additional data should be obtained. However, model results using spatially-averaged values can still be valid and quite helpful for comparing alternatives, for conducting screening-level studies, for identifying data deficiencies, and/or for gaining some general insight into the nature of a problem.

As stated above, the error associated with using an average value versus a spatial distribution is very site specific. For example, the average ground-water velocity over a model region could be the same if the region is simulated with one average value of hydraulic conductivity or if a spatial distribution is used with a range of high and low values. In another similar case, the low values of hydraulic conductivity could be distributed such that they control the flow, and the velocities for the two cases could be very different.

6. How many hydrogeologic layers are to be simulated?

The analyst needs to select a model which can simulate either single or multiple hydrogeologic layers/aquifers depending on the conditions which exist at the site.

Some mathematical models, particularly analytical solutions, can only simulate a single aquifer. The single-aquifer approach is valid for cases where the major portion of the ground-water flow and contaminant transport occurs in a single layer of a multi-layered system, or where the hydraulic properties of all the layers of a multi-layered system are very similar. If the hydraulic properties of the various layers are significantly different and contaminants are being transported in more than one layer, then a multi-layered model should definitely be applied.

Significant differences between geologic layers are difficult to define. For hydraulic conductivities, a significant difference might be anything greater than a factor of 10. Hydraulic gradients and porosity should at a minimum be within a factor of 25%, and flow directions should be essentially the same (both horizontally and vertically). For contaminant transport considerations, the layers should have similar compositions so their sorption properties can accurately be simulated with one value.

7. Do the hydrogeologic layers vary in thickness spatially?

The analyst needs to select a model which can simulate constant or variable thickness hydrogeologic layers depending on the conditions which exist at the site.

Some mathematical models, particularly analytical solutions, can only simulate constant or uniform thickness within a layer or layers. If the thickness of a layer(s) does not change significantly spatially, the uniform assumption is valid. If the thickness changes by more than about 10% of the average thickness, a model should be used that can simulate spatially-variable thickness.

The principle problem associated with not simulating variable thickness is that the transmissivity distribution in the model will be incorrect (transmissivity = hydraulic conductivity x aquifer thickness). Using the wrong transmissivity distribution could have a significant impact on the model results depending on the specifics of the problem being simulated. One of the few ways to determine the magnitude of the impact is to run a sensitivity analysis with site-specific data. In general, changing thicknesses are analogous to changing diameters in pipe flow. Velocities will increase or decrease accordingly, thus affecting travel-time predictions.

8. Is the hydrologic system in a steady-state condition or do water levels fluctuate with time (transient condition)?

The analyst needs to select a model which can simulate the type of hydrologic condition which exists at the site, either steady state or transient.

Steady-state flow is defined as the condition when the magnitude and direction of the flow velocity (as defined by the hydraulic conductivity and hydraulic gradient) are constant with time at any point in the flow field. Transient flow (unsteady flow) is when the magnitude or direction of the flow velocity changes with time at any point in a flow field (Freeze and Cherry, 1979, p.49). The application of a steady-state model or approach is technically valid only in the somewhat unrealistic case where the water table maintains the same position for some extended period of time (throughout the entire simulation period). In most actual cases, variations in recharge and discharge introduce transient effects on the flow system. Therefore, technically speaking, a transient model or approach should always be applied. However, when applying models, the general rule that is followed is that if the fluctuations in the water table are small in comparison with the total vertical thickness of the aquifer (or hydrologic flow system), and if the relative configuration of the water table remains the same throughout the cycle of the fluctuations (i.e., the high and low points remain highest and lowest, respectively), then the transient system can be simulated as a steady-state system with the water table fixed at its mean position. As was the case for confined

versus unconfined flow, small fluctuations in the water table are generally defined as less than about 10% of the total thickness of the aquifer (or flow system).

Transient simulations require much more data and are more difficult to implement than steady-state simulations. Typically, the additional data (time series of water-level measurements, recharge, discharge, etc.) are not available and one is forced to make a steady-state approximation. In many instances the steady-state approach can yield valuable insight and information provided that the assumptions used are conservative and that the limitations of the approach are fully understood.

An approach that can be used to approximate a fully transient simulation but that requires less data and is easier to implement is a series of steady-state solutions. In this approach a new potential or head distribution is solved for whenever a significant stress is imposed on the system. A significant stress can be a pumping well(s) being turned on for a pump-and-treat remedial action, or a cyclic recharge event where it is known, for example, that the majority of the recharge occurs in the winter months.

The errors associated with using a steady-state approximation of a transient system are difficult to quantify because they depend on each specific case. For example, if a water table exhibits very consistent and small fluctuations over a yearly cycle due to a consistent pumping and recharge pattern (i.e., pumping occurs between April and September for

irrigation and natural recharge is large in the winter and small in the summer), a steady-state approximation may be valid. If on the other hand, the pumping schedule is sporadic and it significantly alters hydraulic gradients and directions of flow, and the recharge is variable from season to season and year to year, a transient simulation should be performed.

After these questions (criteria) have been addressed, in most cases the analyst will find that there are several ground-water flow models which meet the desired criteria. At this point the analyst can either select a ground-water flow model and then continue the selection process to choose a compatible (but separate) contaminant transport model, or the user can continue the process to select a combined flow and transport model. It is quite common to find a fairly sophisticated flow model linked with a simpler transport model since the transport model parameters are generally less well known.

The decisions to be made when selecting a contaminant transport model are discussed in more detail below. Some guidance is provided to help in making the decision and some discussion is provided regarding the errors associated with incorrectly using the model or feature(s) of the model.

The errors associated with incorrectly selecting a transport model or feature of a model are difficult to quantify. Some guidance is given below, but in many cases these errors are site specific and, therefore, cannot be quantified in general terms. Following are the questions to be answered when selecting a contaminant transport model.

1. Does the contaminant enter the ground-water flow system at a point or is it distributed along a line or over an area or a volume?

The analyst needs to select a model which can simulate the type(s) of source(s) that exists at the site, either point, line, or area source.

A point source is characterized by contaminants entering the ground water at a single location such as a pipe outflow or injection well. A line source is characterized by contaminants entering the ground water along a line as in the case of leachate emanating from the bottom of a trench. An areal source or nonpoint source is characterized by contaminants entering the ground water over an area as in the case of leachate emanating from a waste lagoon or an agricultural field. A volume source releases contaminants in a form of volume in ground water.

A point source can be simulated with either a one-, two-, or three-dimensional mathematical model whereas a line or areal source should be simulated with a higher dimensional model. Most two- or three-dimensional models can simulate point, line, and areal sources. Three-dimensional models are appropriate for simulating a volume source. All one-dimensional models, particularly analytical solutions, simulate point sources. Line or area sources can be simulated with one-dimensional models by assuming that the contaminant concentration is uniform except in the dimension simulated. Because the analyst typically lacks the necessary data to perform conceptually correct transport simulations, it is quite common to use a one-dimensional transport model with averaged values of

concentration and velocity to simulate line or areal sources. This approach is discussed in more detail below in the section on dimensionality.

Typically, when using a one-dimensional transport model to represent a line or areal source, the plume width is underestimated and its concentration is overestimated. This effect diminishes as the contaminant migrates farther and farther from the source. Also, typically when performing one-dimensional transport simulations, the analyst uses the peak measured concentration in the interest of being conservative. The analyst must keep in mind these conservative aspects of the approach when analyzing the results.

2. Does the source consist of an initial slug of contaminant or is it constant over time?

The analyst needs to select a model which can simulate the type(s) of source release that occurs at the site, either pulse, constant or a combination of both.

Contaminants can enter the ground water either as an instantaneous pulse or as a continuous release over time. A continuous release may be either constant or variable. Variable releases may be due to source decay, variable precipitation on the source, or intermittent source application (e.g., dumping). Many of the simpler mathematical models can only simulate slug or constant input releases. Some of the one-dimensional models and

most of the higher dimensional models can simulate all the various means by which contaminants can enter the ground water.

In many transport modeling studies, a one-dimensional model which cannot properly represent the distribution of the source in time will be used at the screening-level stage to make a conservative prediction of the concentration. The errors associated with simplifying the contaminant input pulse are site specific and, therefore, difficult to quantify. In general, use of a continuous input model will over-predict concentrations if the peak value is set as the input. If an average value is set, the model will under-predict discrete peaks. The effects of using an average flux will diminish with distance from the source.

3. Is it necessary to simulate three-dimensional transport or can the dimensionality be reduced without losing a significant amount of accuracy?

The analyst needs to select a model which can simulate the dimensionality needed to properly represent the site, either one-, two-, or three-dimensional.

All transport models should be selected in three dimensions unless it can be shown that the contaminant migration or remediation scheme can be accurately represented in a lower dimension. Cases where a contaminant source is distributed both areally (x-y) and vertically (z) would, in most instances, require a fully three-dimensional model. Similarly, remedial action simulations employing pumping wells screened at specified depths and/or cutoff walls not fully penetrating an aquifer would most likely

require a three-dimensional model. Cases in which the aquifer is uniformly contaminated in the vertical direction and where geologic layering is not important can be simulated in two dimensions, generally either in x-y or x-z. Very simple cases consisting of a large plane source, a simple contaminant distribution, and a uniform velocity distribution can be simulated with a one-dimensional model.

Because the analyst typically lacks the necessary data to develop a two- or three-dimensional transport model, it is quite common to simulate transport in one dimension. Only in recent years have documented and verified three-dimensional models become available,and responsible parties have been willing to spend the time and money required to develop and run site-specific models. The lack of necessary data is no excuse for running a lower dimensional model if it is not suited for the specific application, although this is the approach which apparently is often taken. A one-dimensional model, however, can still provide valuable results for a screening study where conservative predictions or alternatives are compared.

The limitations of the one-dimensional approach are:

- it cannot simulate multiple sources;
- it can only simulate a large plane source or an average concentration distribution over a large x-y, x-z, or y-z plane for an areal source; and

- it cannot simulate transverse dispersion (perpendicular to the flow path).

Although errors associated with these limitations are difficult to quantify, their general effect is the prediction of very conservative (higher) concentrations. A conservative prediction can be useful for screening studies, but often the results are so conservative that they have little use.

The dimensionality of the transport model should be equal to or less than the dimensionality of the ground-water flow model. Although it is possible to simulate the ground-water flow with a one-dimensional model and then simulate contaminant transport with a three-dimensional model, the transport simulation would not truly be a three-dimensional simulation since the flow vector is in only one direction.

It is important to remember that performing a complete three-dimensional analysis does not by any means eliminate uncertainty in the results. It is virtually impossible to completely characterize a ground-water flow/contaminant transport system, and no matter how well the system is characterized, the model, whether one-, two-, or three-dimensional, is always a simplified representation of the real system. Three-dimensional model results, as well as one- and two-dimensional model results, need to be analyzed very carefully to make sure they are reasonable.

4. Does the model simulate dispersion?

Dispersion is the spreading of a solute in porous medium caused by mechanical mixing of water through the media. Dispersion cannot be expressed in terms of the mean ground-water velocity alone. Local variations in flow velocity direction and magnitude caused by the natural heterogeneity in media properties causes dispersion. The spreading process is usually associated with unknown and uncharacterized geologic variation of hydraulic properties. The dominant property causing the spreading is usually the hydraulic conductivity variation in space(Simmons and Cole, 1985).

Most all contaminant transport models simulate some form of dispersion. There is much concern, however, as to whether dispersion can be adequately described in a model because it is related to spatial scale and variations in hydraulic properties which are difficult to simulate in a model. There seems to be a clear consensus among ground-water transport researchers that the conventional convective-dispersive equation may be an inadequate and inappropriate description of field-scale dispersion (Pickens and Grisak 1981a and b; Jury 1982; Smith and Schwartz 1980; Gelhar et al. 1979; Matheron and DeMarsily 1980; Dagan and Bresler 1979; Simmons 1982a and b). Some recognized inadequacies of the conventional approach are prediction of non-physical upstream migration, failure to predict increased dispersion caused by larger scales of heterogeneity, inappropriate dependence on diffusion-like boundary conditions, and incorrect representation of non-Fickian, asymmetric solute distributions (Simmons and Cole, 1985). For

the purposes of this report, it will be assumed that the currently available models are adequate.

It is difficult to quantify the errors associated with simulating dispersion because they are site specific. Turning off dispersion in a model only considers the movement of contaminants by the advection process and hence yields a "worst case" prediction of peak contaminant concentration. However, this causes the leading edge of the plume to take longer to arrive at a point downgradient. The larger the value of dispersion, the greater the spread of the plume and the lower the peak concentration. Since dispersion coefficients are very difficult to measure in the field, the best way to choose a value is in the model calibration process, often requires a large amount of data for field calibration.

5. Does the model simulate adsorption (i.e., distribution or partitioning coefficient) and, if so, does it simulate temporally and/or spatially variable adsorption? Temporally or spatially variable adsorption is important when the soil conditions and/or concentrations change with time and space.

There are a number of chemical and biological processes that affect the rate and manner in which contaminants travel in the ground water (adsorption, ion exchange, degradation, biotransformation, etc.). Since adsorption and degradation (decay) are the only processes that are typically simulated in contaminant transport models, they are the only processes discussed in this report. Adsorption is discussed in this section and degradation in the next section.

Adsorption is usually represented by a distribution or partitioning coefficient which relates contaminant concentration in solution to contaminant concentration associated with (adsorbed to) the soil. Distribution coefficients are used in transport models to approximate contaminant retardation in the subsurface. Contaminant retardation relates ground-water velocity to contaminant velocity.

In screening studies, transport models not simulating adsorption are often used to make conservative estimates of contaminant concentrations. These conservative estimates can be useful as long as the predicted concentrations are not so high that they completely misrepresent the problem. A general rule for determining when to simulate adsorption might be that if the contaminant is only mildly retarded, say less than a factor of 5 times slower than the ground water, then the conservative approach of not simulating adsorption may be informative in a screening effort. If the contaminant has a retardation factor larger than 5, a model should be selected that simulates retardation. In any detailed modeling study adsorption should always be simulated for all retarded contaminants. The partitioning coefficients for all contaminants are dependent on the equilibrium solution concentration. However, in dilute solutions, the partitioning coefficient is constant for all practical purposes (linear isotherm). Stated in a different way, a contaminant's absorption properties remain the same at low concentrations (linear), whereas at higher concentrations adsorption decreases as the contaminant concentration in the ground water increases (nonlinear). This nonlinear property can become very important when predicting the migration of the center of mass

versus the leading edge of a contaminant plume, or when predicting required pumping time for a pump-and-treat remedial action. At high concentrations, the linear assumption will over-predict adsorption and travel times and under-predict ground-water contaminant concentrations. For hydrophobic contaminants, the threshold below which linearity can be assumed is about one half the solubility (Neely and Blau, 1985). For hydrophilic substances, the threshold must be determined on a case-by-case basis because of interactions between the water and the contaminant.

Very few currently available transport models can simulate the nonlinear adsorption case, so adsorption is nearly always simulated as a linear isotherm. For very low concentrations, this approximation can produce mass balance errors which typically overestimate the contaminant mass in the solution phase and underestimate the mass in the solid phase. Therefore, the approximation with the linear isotherm is more conservative (i.e., it would predict a higher concentration at a monitoring well at an earlier time than it should actually arrive).

Certainly, it would be more accurate to use a nonlinear isotherm model for all cases in which it applies. The currently accepted practice in transport modeling, however, is to lump all chemical and biological processes into one term, the adsorption or retardation term, and simulate it as a linear isotherm. Geochemical models are employing a more state-of-the-art approach with regard to simulating chemical and biological processes. Until the science is better understood, however, the accepted practice will be to lump them all into one term.

6. Does the model simulate first or second-order decay and/or radionuclide decay?

Degradation or radionuclide decay are factors which can significantly affect predicted concentrations and total mass of contaminants in a ground-water system. As with adsorption, conservative estimates of concentrations can be made by neglecting degradation in a screening level or "worst-case" analysis. For a detailed analysis, however, a degradation model should be used.

Most transport models simulate first-order decay. Only a few models can simulate higher-order decay. No transport models are currently available which can simulate the transformation of one chemical constituent into a breakdown product and then simulate the transport of the transformed constituent(s). One approach that can be used to simulate the transport of a parent species and all its transformation products is to simulate the transport of a parent as if there is no degradation and then apportion the resulting concentration on the basis of an assumed transformation efficiency (often 10%) and the ratio of molecular weight. This only works well if the adsorption coefficients are similar between the parent and by-product contaminants. It also assumes that the by-product does not further transform.

Several transport models, both analytical and numerical, can simulate radioactive decay. Many of the models can account for the generation and transport of daughter products in both straight and branched decay chains.

7. Does the model simulate density effects due to changes in temperature and concentration? A truly coupled model is one in which the ground-water flow is influenced by the density and viscosity of the water, which, in turn, are influenced by the temperature of the water and the concentration of the solute. In some cases (i.e., involving a large heat source or large fluctuations in solute concentration) it may be important to consider temperature and contaminant concentration effects on ground-water flow.

A basic assumption of most ground-water flow and contaminant transport models is that gradients of fluid density, viscosity, temperature, and concentration do not affect the velocity distribution. In most cases these gradients are small and this is a safe assumption. In some cases, however, these gradients can become large and can significantly affect flow patterns. In these cases a coupled model solving for pressure, temperature, and/or solute concentration as functions of fluid density and viscosity should be used.

An example of such a case is the effect of heat generated by the burial of high-level radioactive waste on the ground-water flow in the vicinity of the repository. The heat from the repository will have a buoyant effect on the surrounding water causing it to rise. The extent of the rise and the magnitude of the impact can be predicted with coupled models.

Under most naturally-occurring situations, the assumption that flow is not affected by temperature, density, and concentration gradients is valid. In cases where extremely deep systems are being simulated, however, the naturally-occurring geothermal gradients may influence ground-water flow patterns and should therefore be simulated. The only other cases where one

typically needs to be concerned with thermal flow patterns are anthropogenic phenomenon such as geologic repositories or injection of heated or cooled fluids.

Similarly, under most naturally occurring circumstances, density and concentration gradients are small enough they can be neglected. The classic example of a naturally-occurring density problem that should be simulated with a coupled model is that of saltwater intrusion. Most man-made contamination problems result in low enough ground-water concentrations that they do not affect the ground-water flow. In a few instances, concentrations become large enough that the density of the water is affected and a coupled model is required for an accurate prediction of the flow and transport. An important example is leachate from landfills. Concentrated leachate plumes often move deep into the aquifer before they migrate laterally. If the effect of concentration is neglected, the analysis may under-predict concentration at deeply screened wells.

After sequencing through the decision tree, there will, in most cases, be several models which meet the desired criteria. Since several models could meet the desired criteria, it is difficult to list a single model as a standard model. At this point the analyst can either select a transport model which is compatible with the flow model selected above, or select a combined ground-water flow/contaminant transport model.

Regardless of the approach selected, whether separate or combined flow and transport models, it is likely that there will be several models which meet the technical criteria. The selection of the final model(s) should be based on the

implementation criteria; i.e., the model meets the criteria that it has been through a rigorous quality assurance program so that it is thoroughly verified, and the model is well documented with user's manuals and test cases.

If several models pass the quality assurance and documentation criteria, the final selection of a model should be based on familiarity with and availability of the model, the modeling schedule, available budget, and staff and equipment resources.

5.2. MODEL SELECTION FROM THE REVIEWERS POINT OF VIEW

The selection criteria are described primarily from the point of view of an analyst performing an exposure assessment study. The basic process begins with defining project objectives, assessing a physical situation, and then selecting a model to represent the important processes relevant to the objectives and physical conditions. Another use of the selection criteria is from the point of view of a regulatory agency that is reviewing an exposure assessment study. Under these circumstances the reviewer needs to evaluate the choice of the model used in performing the study. The selection criteria must be fundamentally the same for both applications, however, some differences exist in how the criteria is used or evaluated. This section is included to describe those differences. The proper selection of a model is one step in performing an exposure assessment study. All models are sensitive to the choice of input parameters. The choice of these parameters will be, in most cases, at least as important as the choice of a particular model and must be considered in the review process.

The first step for the person reviewing the exposure assessment study is to identify the characteristics and capabilities of the specific model. This information can best be obtained from a model user's manual.

The single most important step in choosing a model is to define project objectives. Similarly, the most important step for the reviewer is to have a clear understanding of the study objectives. The objectives of the analysis should clearly state whether it is performed as a generic analysis or if a more detailed site-specific analysis with appropriate data for calibration and validation is intended. In cases where the objectives are not clearly defined, then the only option is to interpret how the results and conclusions of the study are presented (e.g., associated uncertainty, potential impacts, and importance of decisions based on the results). This is difficult and will obviously be subjective in some cases. After this initial step, the rest of the selection criteria are essentially the same for both the selection of a model and review of a model selection by another person.

It is important that the reviewer examine the presentation of results and conclusions to see that they are consistent with the study objectives, model choice, and model application. Any decisions based on model results must incorporate the uncertainty inherent in the predictions. For a generic analysis, the level of uncertainty will be about an order of magnitude at best. For more detailed analysis, the validation phase of a modeling study may provide some guidance in defining the uncertainty associated with the model predictions.

5.3. MODEL SELECTION WORKSHEET

Section 5.1 discussed the technical criteria used to select a mathematical model for a specific application. This section provides a model selection worksheet which facilitates the selection of an actual model or suite of models based on the response to the technical criteria.

The model selection worksheets are shown in Tables 5-1, 5-2, and 5-3. Tables 5-1 and 5-2 are the analytical solutions worksheets and Table 5-3 is the analytical and numerical model (coded for the computer) worksheets.

Table 5-1 lists a total of 63 analytical solutions by name and reference, tells which calculator or personnel computer they have been programmed for (if any), and lists any pertinent comments. The first seven solutions are for ground-water mounding problems and the remainder are for contaminant transport problems.

Table 5-2 lists the analytical solutions (by number) in the same order they are listed in Table 5-1. The technical selection criteria (listed across the top) are in the same order as they are discussed in Section 5.1 (Figure 5-1).

Table 5-3 presents a list of some of the currently available, documented, mathematical models. The models are divided into seven categories:

1. Analytical flow models
2. Analytical transport models
3. Numerical flow models which can be applied to both saturated and unsaturated systems
4. Numerical flow models which can only be applied to saturated systems
5. Numerical contaminant transport models which can be applied to both saturated and unsaturated systems
6. Numerical contaminant transport models which can only be applied to saturated systems
7. Numerical contaminant and transport models which couple the solutions for pressure, temperature, and concentration (coupled models).

Within these major categories, the models are listed in alphabetical order. The technical criteria or specifications for the models (listed across the top) are

TABLE 5-1. ANALYTICAL SOLUTIONS, NAMES, AND REFERENCES

Analytical Solution Name	Computer Type	Comments	Reference
1) Analysis of Groundwater Mounding Beneath Tailings Ponds	TI-88	Predicts Hydraulic Head	Sandberg et al., 1981 Prickett and Verhoes, 1981
2) Circular Recharge Area	TI-59	Predicts Hydraulic Head	Walton, 1983
3) Circular Basin Recharge Mound	HP-41	Predicts Hydraulic Head	Ulrick (1)
4) Mound Decay		Predicts Hydraulic Head	Bear, 1972
5) Circular Recharge Area	TRS-80, Osborne, Kaypro, IBM	Predicts Hydraulic Head	Walton, 1983
6) Mounding	Apple, Victor, Kaypro II, Vector	Predicts Hydraulic Head	(2)
7) Glover's Solution	Apple	Predicts Hydraulic Head and Discharge	Walden, Sananda, and Warner, 1984
8) Advection and Dispersion -- Regional Flow	(3)	Predicts Contaminant Concentration	Walton, 1983
9) MAP PLUME	Apple, Victor, Kaypro II, Vector	Predicts Contaminant Concentration	(2)
10) PLUME	Osborne, Super-brain, Kaypro, IBM	Predicts Contaminant Concentration	(2) (4)
11) PLOSBNB	Osborne	Predicts Contaminant Concentration	(5)
12) PLUME CROSS-SECTION	Apple, Victor, Kaypro II, Vector	Predicts Contaminant Concentration	(2)
13) RANDOM WALK	(6)	Predicts Contaminant Concentration	(2)
14) RANDOM WALK	(7)	Predicts Contaminant Concentration	(3)
15) RWOSBNB	Osborne	Predicts Contaminant Concentration	(5)
16) SWMY	Osborne	Predicts Contaminant Concentration	(5)
17) Advection and Dispersion from a Stream	TRS-80, (3)	Predicts Contaminant Concentration	Walton, 1983
18) Advection and Dispersion from a Single Pumping Well	TRS-80, (3)	Predicts Contaminant Concentration	Walton, 1983
19) Advective Mass Transport Thats Particle Mover	TI-59	Predicts Contaminant Concentration	Sandberg et al., 1981 Prickett and Verhoes, 1981
20) Streamlines and Travel Times for Regional Flow Affects by Sources and Sinks	HP-41	Particle Location with Time	Olsthoorn, 1984 (4)
21) Advective Transport Model	HP-41	Particle Location with Time	Ulrick, 1983 (1)
22) 3-Paths	HP-41	Predicts Mass Loading	Oberlander and Nelson, 1984
23) Ground Water Dispersion	TI-58/59	Predicts Contaminant Concentration	Kelly, 1982
24) Plume Management Model	TI-59	Predicts Contaminant Concentration	Sandberg et al., 1981 Prickett and Verhoes, 1981
25) Calculator Code for Evaluation Landfill Leachate Plumes	TI-59	Predicts Contaminant Concentration	Pettyjohn et al., 1982
26) Dissipation of a Concentrated Slug of Contaminant	TI-69	Predicts Contaminant Concentration	T.A. Prickett and Associates (8)
27) Advection and Dispersion from a Single Solute Injection Well	HP-41	Predicts Contaminant Concentration	Van der Heijde, 1984 (4)
28) GBAST -- Analytical Solution for One-Dimensional Contaminant Transport		Predicts Contaminant Concentration	Javandel et al., 1984
29) TBAST -- Analytical Solution for Two-Dimensional Contaminant Transport		Predicts Contaminant Concentration	Javandel et al., 1984
30) LTBRD -- Semi-Analytical Solution to Radial Dispersion in Porous Media		Predicts Contaminant Concentration	Javandel et al., 1984
31) GESSQ -- Semi-Analytical Contaminant Transport		Predicts Contaminant Concentration	Javandel et al., 1984
32) GT -- Mapping Concentration Distribution in an Aquifer Based on a Time Series Data Collection Concept		Predicts Contaminant Concentration	Javandel et al., 1984
33) Material Release on the Surface with One-Dimensional Vertical Downward Transport		Predicts Contaminant Concentration	vanGenuchten and Alves, 1982 (9)
34) Two-Dimensional Horizontal Flow with a Slug Source		Predicts Contaminant Concentration	Wilson and Miller, 1978 (9)
35) Two-Dimensional Horizontal Flow with a Continuous Source		Predicts Contaminant Concentration	Wilson and Miller, 1978 (9)
36) Instantaneous Source, Infinite Aquifer Depth		Point Source Solution	Kwang, 1986
37) Instantaneous Source, Finite Aquifer Depth		Point Source Solution	Kwang, 1986
38) Instantaneous Source, Finite Aquifer Depth -- Average Concentration		Point Source Solution	Kwang, 1986
39) Continuous Source Release -- Unsteady State		Point Source Solution	Kwang, 1986
40) Continuous Source Release -- Steady State		Point Source Solution	Kwang, 1986
41) Instantaneous Horizontal Release, Finite Source Length, Infinite Aquifer Depth		Line Source Solution	Kwang, 1986
42) Instantaneous Horizontal Release, Infinite Source Length, Infinite Aquifer Depth		Line Source Solution	Kwang, 1986

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TABLE 5-1. (continued)

Analytical Solution Names	Computer Type	Comments	Reference
43) Instantaneous Horizontal Release, Finite Source Length, Finite Aquifer Depth		Line Source Solution	Hwang, 1986
44) Instantaneous Horizontal Release, Finite Source Length, Aquifer Depth-Averaged Concentration		Line Source Solution	Hwang, 1986
45) Continuous Horizontal Release, Finite Source Length, Infinite Aquifer Depth		Line Source Solution	Hwang, 1986
46) Instantaneous Vertical Release, Infinite Aquifer Depth		Line Source Solution	Hwang, 1986
47) Continuous Vertical Release, Average Concentration -- Unsteady State		Line Source Solution	Hwang, 1986
48) Continuous Vertical Release, Average Concentration -- Steady State		Line Source Solution	Hwang, 1986
49) Instantaneous Horizontal Source		Areal (Plane) Source Solution	Hwang, 1986
50) Instantaneous Vertical Source		Areal (Plane) Source Solution	Hwang, 1986
51) Continuous Horizontal Plane Source -- Unsteady State		Areal (Plane) Source Solution	Hwang, 1986
52) Continuous Horizontal Plane Source -- Steady State		Areal (Plane) Source Solution	Hwang, 1986
53) Continuous Vertical Plane Source -- Unsteady State		Areal (Plane) Source Solution	Hwang, 1986
54) Horizontal Plane Source at a Constant Boundary Concentration		Areal (Plane) Source Solution	Hwang, 1986
55) Vertical Plane Source at a Constant Boundary Concentration -- Steady State		Areal (Plane) Source Solution	Hwang, 1986
56) Constant Release Rate Downward		Infinite Horizontal Plane Source	Hwang, 1986
57) Constant Concentration Boundary Reservoir		Infinite Vertical Plane Source	Hwang, 1986
58) Volume Source			Hwang, 1986
59) Constant Boundary Concentration in a Radially-Flowing Aquifer			Hwang, 1986
60) One-Dimensional Mass Transport	IBM 360/91	Concentration and Flow Boundary Conditions	Cleary and Ungs, 1978
61) Two-Dimensional Mass Transport	IBM 360/91	Strip Boundary Condition Finite and Infinite Width	"
62) Three-Dimensional Mass Transport: Patch Source; Finite Dimensions	IBM 360/91	Two-Dimensional Vertical Source	"
63) Three-Dimensional Mass Transport: Bivariate Gaussian Source	IBM 360/91		"

(1) Programs available from James S. Ulrick and Associates, 2100 Los Angeles Avenue, Berkeley, CA 94707.

(2) Programs available from the National Center for Ground Water Research, Oklahoma State University, Stillwater, OK.

(3) Calculator/Computer Type: Osborne, Kaypro, Superbrain, IBM, Radio Shack PC-1 and PC-2, and Sharp PC 1250 and 1500 programs available.

(4) Programs available from the International Ground Water Modeling Center, Holcomb Research Institute, Butler University, 4600 Sunset Avenue, Indianapolis, IN 46208.

(5) Programs available from Dr. Michael L. Voorhees of Warzyn Engineering, Inc., Madison, WI.

(6) Calculator/Computer Type: Apple, Kaypro II, Victor, Vector, TRS-80, Sharp-PC1600.

(7) Calculator/Computer Type: Superbrain, Osborne, Sharp-PC1600.

(8) Programs available from Thomas A. Prickett and Associates, Inc., 8 Montclair Road, Urbana, IL 61801.

(9) See National Council of the Paper Industry for Air and Stream Improvements, Inc., Technical Bulletin No. 472, October, 1985.

P -- Point Source
L -- Line Source
A -- Areal Source
R -- Radial Flow
x -- x-Dimension
y -- y-Dimension
z -- z-Dimension
Vol -- Volume
D_x -- Dispersion in the x Direction
D_y -- Dispersion in the y Direction
D_z -- Dispersion in the z Direction

TABLE 5-2. ANALYTICAL SOLUTIONS WORKSHEET

Analytical Solutions No. (see Table 1)	Water Table Aquifer	Confined Aquifer	Porous Media	Fracture Flow	Flow Dimension	Single-Phase	Multi-Phase	Homogeneous Hydraulic Parameters	Heterogeneous Hydraulic Parameters	Single-Layer	Multi-Layer	Constant Thickness	Variable Thickness	Steady State	Transient	Point, Line, Areal Source	Initial Value Source	Constant Source	Dispersion	Adsorption	Degradation 1,2,-Order Radioactive
Groundwater Mounding																					
1	X		X		R	X		X		X		X			X	Circ	X		X		
2	X		X		R	X		X		X		X			X	Circ	X		X		
3	X		X		R	X		X		X		X			X	Circ	X		X		
4	X		X		X-Y	X		X		X		X			X	Rect	X		X		
5	X		X		R	X		X		X		X			X	Circ	X		X		
6	X		X		R	X		X		X		X			X	Circ	X		X		
7	X		X		R	X		X		X		X			X	Rect	X		X		
Contaminant Transport																					
8		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
9		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
10		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
11		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
12		X	X		X-Z	X		X		X		X			X	P	X		X	X	X
13	X	X	X		X-Y	X		X		X		X			X	P	X		X	X	X
14	X	X	X		X-Y	X		X		X		X			X	P	X		X	X	X
15		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
16	X	X	X		X-Y	X		X		X		X			X	P	X		X	X	X
17		X	X		X	X		X		X		X			X	P	X		X	X	
18		X	X		R	X		X		X		X			X	P	X		X	X	
19		X	X		X-Y	X		X		X		X			X	P	X		X		
20		X	X		X-Y	X		X		X		X			X	P	X		X		
21		X	X		X-Y	X		X		X		X			X	P	X		X		
22		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
23		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
24		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
25		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
26		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
27		X	X		R	X		X		X		X			X	P	X		X		
28		X	X		X	X		X		X		X			X	P	X	X	X	X	X
29		X	X		X-Y	X		X		X		X			X	LS	X	X	X	X	X
30		X	X		R	X		X		X		X			X	P		X	X		
31		X	X		X-Y	X		X		X		X			X	P,A		X		X	
32		X	X		R	X		X		X		X			X	P	X	X	X	X	

TABLE 5-2. (continued)

Analytical Solutions No. (see Table 1)	Water Table Aquifer	Confined Aquifer	Porous Media	Fracture Flow	Flow Dimension	Single-Phase	Multi-Phase	Homogeneous Hydraulic Parameters	Heterogeneous Hydraulic Parameters	Single-Layer	Multi-Layer	Constant Thickness	Variable Thickness	Steady State	Transient	Point, Line, Areal Source	Initial Value Source	Constant Source	Dispersion	Adsorption	Degradation 1,2,-Order Radioactive
33			X		Z	X		X		X		X			X	P		X	X	X	X
34		X	X		X-Y	X		X		X		X			X	P	X		X	X	X
35		X	X		X-Y	X		X		X		X			X	P		X	X	X	X
Transport																					
36		X	X		X-Y-Z	X		X		X		X			X	P	X		X	X	X
37		X	X		X-Y-Z	X		X		X		X			X	P	X		X	X	X
38		X	X		X-Y-Z	X		X		X		X			X	P	X		X	X	X
39		X	X		X-Y-Z	X		X		X		X			X	P		X	X	X	X
40		X	X		X-Y-Z	X		X		X		X		X		P		X	X	X	X
41		X	X		X-Y-Z	X		X		X		X			X	L	X		X	X	X
42		X	X		X-Y-Z	X		X		X		X			X	L	X		X	X	X
43		X	X		X-Y-Z	X		X		X		X			X	L	X		X	X	X
44		X	X		X-Y-Z	X		X		X		X			X	L	X		X	X	X
45		X	X		X-Y-Z	X		X		X		X			X	L		X	X	X	X
46		X	X		X-Y	X		X		X		X			X	L	X		X	X	X
47		X	X		X-Y	X		X		X		X			X	L		X	X	X	X
48		X	X		X-Y	X		X		X		X		X		L		X	X	X	X
49		X	X		X-Y-Z	X		X		X		X			X	A	X		X	X	X
50		X	X		X-Y-Z	X		X		X		X			X	A	X		X	X	X
51		X	X		X-Y-Z	X		X		X		X			X	A		X	X	X	X
52		X	X		X-Y-Z	X		X		X		X		X		A		X	X	X	X
53		X	X		X-Y-Z	X		X		X		X			X	A		X	X	X	X
54		X	X		X-Y-Z	X		X		X		X			X	A		X	X	X	X
55		X	X		X-Y-Z	X		X		X		X		X		A		X	D_z D_y	X	X
56		X	X		Z	X		X		X		X			X	A		X	D_z	X	X
57		X	X		X	X		X		X		X			X	A		X	D_x	X	X
58		X	X		X-Y-Z	X		X		X		X			X	Vol	X	X	X	X	X
59	X	X	X		R	X		X		X		X			X	P,A		X	X	X	X
60	X		X		Z	X		X		X		X			X	P		X	X	X	X
61		X	X		X-Y	X		X		X		X			X	A		X	X	X	X
62	X		X		X-Y-Z	X		X		X		X			X	A		X	X	X	X
63	X		X		X-Y-Z	X		X		X		X			X	Vol		X	X	X	X

TABLE 5-2. (continued)

LEGEND

Dimension

X -- X dimension
Y -- Y dimension
Z -- Z dimension

Dispersion

D_x -- Dispersion in x direction
D_y -- Dispersion in y direction
D_z -- Dispersion in z direction

R -- Radial Flow

Source Type

A -- Areal source
L -- Line source
P -- Point source

Vol -- Volume

TABLE 5-3. ANALYTICAL AND NUMERICAL MODELS WORKSHEET

Model Names	Water Table Aquifer	Confined Aquifer	Porous Media	Fracture Flow	Dimension Flow	Single-Phase	Multi-Phase	Homogeneous Hydraulic Parameters	Heterogeneous Hydraulic Parameters	Single-Layer	Multi-Layer	Constant Thickness	Variable Thickness	Steady State	Transient	Point, Line, or Areal Source	Initial Value Source	Constant Source	Dimension Transport	Dispersion	Adsorption	Degradation 0,1,2-Order Radioactive	Density Effects	Solution Technique
Analytical Flow																								
PATHS		X	X		2	X		X		X		X		X	X	A	X	X	2		X			AN
Analytical Transport																								
AT123D			X		1,2,3	X		X		X		X		X		A	X	X	1,2,3	X		1		AN
CHAIN			X		1	X		X		X		X		X		P	X	X	1	X	X	1,R		AN
GETOUT			X		1	X		X		X		X		X		P		X	1	X		1,R		AN
GWMTM1&2			X		1,2	X		X		X		X		X		P,L		X	1,2	X		1		AN
NUTRAN			X		1,2,3	X			X	X		X		X		P,L,A		X	1,2,3	X	X	R		AN
NWFT/DVM			X		1	X			X	X		X		X				X	1	X	X	R	Salt	AN
Numerical Flow (Saturated/Unsaturated)																								
UNSAT1			X		1	X			X		X		X		X									FE
FEMWATER1			X		2	X		X	X	X	X	X	X	X	X									FE
UNSAT2			X		2	X			X		X		X		X									FE
FREEZE	X	X	X		3	X			X		X		X		X									FD
Numerical Flow (Saturated Only)																								
BEWTA	X		X		2	X		X		X		X			X									FD
COOLEY	X	X	X		2	X			X	X		X		X	X									FE
FE3DGW	X	X	X		3	X			X		X		X	X	X									FE
FLUMP	X		X		2	X			X	X		X		X	X									FE
FRESURF 1&2	X		X		2	X			X	X	R-Z X	X	R-Z X		X									FE
TERZAGI	X		X		3	X			X		X		X		X									FD
USGS2D	X	X	X		2	X			X	X		X			X									FD
VTT	X	X	X		2	X			X		X		X	X	X									FD
V3	X	X	X		2	X			X		X		X		X									FD
USGS3D-Modular	X	X	X		3	X			X		X		X	X	X									FD
USGS3D-Trescott	X		X		3	X			X		X		X	X	X									FD
Numerical Transport (Saturated/Unsaturated)																								
FEMWASTE1	X		X		2	X			X	X	X	X	X	X	X	A	X	X	2	X	X	1		FE
PERCOL	X		X		1	X	X				X		X	X	X	P	X		1	X	X	R		MR

TABLE 5-3. (continued)

Model Names	Water Table Aquifer	Confined Aquifer	Porous Media	Fracture Flow	Dimension Flow	Single-Phase	Multi-Phase	Homogeneous Hydraulic Parameters	Heterogeneous Hydraulic Parameters	Single-Layer	Multi-Layer	Constant Thickness	Variable Thickness	Steady State	Transient	Point, Line, or Areal Source	Initial Value Source	Constant Source	Dimension Transport	Dispersion	Adsorption	Degradation 0,1,2-Order Radioactive	Density Effects	Solution Technique
SATURN	X		X		2	X			X		X		X	X	X	A	X	X	2	X	X	1,R		FE
SEGOL	X		X		3	X			X		X		X	X	X	A	X	X	3	X	X			FE
SUMATRA-I	X		X		1	X			X		X		X	X	X	P	X	X	1	X	X	0,1	X	FE
SUTRA	X		X		2	X			X		X		X	X	X	A	X	X	2	X	X	1	X	FE, IFD
TRANUSAT	X		X		1,2	X			X		X		X	X	X				1,2	X	X	1		FE
TRUST	X		X		1,2,3	X			X		X		X	X	X	P,L,A	X	X	1,2,3	X	X			FD
Numerical Transport (Saturated Only)																								
CHAINT			X	X		X		X		X		X			X	A	X	X	2	X	X	R,CH		FE
DUGUID-REEVES			X			X			X	X	X		X	X	X	A	X	X	2	X	X	R		FE
GROVE/GALERKIN			X		3	X			X		X		X	X	X	A	X	X	3	X	X	1		FE
ISOQUAD,ISOQUAD2			X			X			X	X		X		X	X	A		X	2	X				FE
CONBRED (USGS2D-MOC)					1,2				X	X			X	X	X	A		X	1,2	X	X	1		FD, RW
DPCT	X		X		2	X			X		X		X	X	X	A	X	X	2	X	X	R		FE, RW
MMT			X			X		X		X		X		X	X	P	X	X	1	X		I,R, CH		RW
PINDER		X	X			X			X		X		X	X	X	A		X	3	X	X			FE
ROBERTSON1	X		X			X			X		X		X	X	X	P			2	X		R		FD
ROBERTSON2		X	X		2	X			X	X		X		X	X	A		X	2	X	X	R		FD, MOC
SWENT		X	X		1,2,3	X			X		X		X	X	X	A			1,2,3	X	X	1,R, CH	X	FD
TRANS (Prickett-Lonnquist)	X	X	X		2	X		X		X		X		X	X	A			2	X		1		RW
TRANSAT2		X	X		3	X			X		X		X	X	X				3	X	X	1		FE
Numerical Coupled Solute and Heat Transport																								
CFEST		X	X		1,2,3	X			X		X		X		X	A	X	X	1,2,3	X	X	1	X	FE
GWTHERM			X		2	X			X		X		X		X	A	X	X	2	X	X		X	FD
OCRE			X		1,2	X		X			X	X			X	A		X	1,2	X	X	R		FE
SHALT			X		2	X			X		X		X		X	A		X	2	X	X	1	X	FE
SWIFT	X	X	X		3	X			X		X		X	X	X	A		X	3	X	X	R,CH	X	FD
SWIP2	X	X	X		3	X			X		X	X			X	A	X		3	X	X	1	X	FD

TABLE 5-3. (continued)

LEGEND

AN -- Analytical

Degradation

0 -- Zero Order Decay
1 -- First Order Decay
2 -- Second Order Decay
R -- Radioactive Decay
CH -- Radioactive Chain Decay

Dimensionality

1 -- One Dimensional
2 -- Two Dimensional
3 -- Three Dimensional

FD -- Finite Difference
FE -- Finite Element
IFD -- Integrated Finite Difference
MOC -- Method of Characteristics
NR -- Newton-Raphson

Source Type

A -- Areal Source
L -- Line Source
P -- Point Source

identified in the same order as the technical selection criteria discussed in Section 5.1 (Figure 5-1). The last column in the worksheet includes comments pertaining to the solution technique (analytical model, finite difference, or finite element numerical model) and any other pertinent information. A summary of each of the models listed in Table 5-3 is contained in Appendix A. More detailed information, user's manuals, and copies of many of these models can be obtained from the International Ground Water Modeling Center (IGWMC) model data base. IGWMC is located in Indianapolis, Indiana.

In many instances, selection of a model that has more capabilities than necessary but with which the analyst is familiar may be more cost effective than applying a smaller, unfamiliar model with minimum capabilities due to the acquisition, testing, and learning process that would be required.

5.4. WASTE MANAGEMENT MODELS

A few models have been developed by/for the EPA and others which consist of a methodology for tracing contaminant movement through the various environmental media. For the purposes of this report, these models will be called waste management models. Waste management models typically track the movement of hazardous waste from the source (point of disposal) through one or more of the three primary environmental pathways; air, surface water, and/or ground water. Since this document is concerned with ground-water models, we will only discuss those waste management models which simulate the ground-water pathway.

Waste management models typically consist of a number of submodels to simulate the many components of transport from a contaminant source to the point of exposure. These submodels usually consist of 1) source term generation, which can include leakage through a liner(s); 2) contaminant transport through the unsaturated zone; 3) contaminant transport through the saturated zone; and

4) uptake by humans at the point of exposure. When simulating contaminant transport, the submodel generally simulates phenomena such as dispersion, degradation, and adsorption.

It is not the objective of this document to cover waste management models in any detail. Rather, a few such models are described briefly to make the reader aware of them. If a waste management model uses a ground-water transport model that was discussed earlier, this is brought to the attention of the reader.

5.4.1. Risk Assessment Methodology for Regulatory Sludge Disposal Through Land Application

ICF Technology, Inc., has recently developed a risk-based approach to setting sludge criteria for land application disposal for the EPA. The methodology can also be applied on a site-specific basis to evaluate permit applications. ICF developed the modules addressing ground water, vapor, and surface runoff pathways. In each case, analytical models were assembled to track the movement of contaminants from source to site of exposure. Predicted levels can be compared to health-based criteria, or health-based criteria can be input to select limiting sludge contaminant concentration criteria. A series of representative scenarios are being evaluated with the methodology to identify criteria thresholds and areas where best management practices should be prescribed.

5.4.2. Risk Assessment Methodology for Regulating Landfill Disposal of Sludge

ICF Technology, Inc., has been responsible for the development of the risk-based methodology for EPA upon which sludge landfill disposal regulations and criteria are being based. The methodology can be applied on a national/regional level or on a site-specific basis. For the ground-water

pathway, it predicts leachate quantity and quality and subsequent impacts on ground water by modeling contaminant movement through the unsaturated zone and in the aquifer. Degradation, adsorption, and geochemistry are all accounted for. A simple vapor-release and atmospheric-dispersion approach is taken for the vapor pathway. Runoff and particulate suspension are addressed through best management practices.

The landfill disposal methodology uses the CHAIN model and the AT123D model to simulate contaminant transport through the unsaturated and saturated zones, respectively. Both of these models are discussed in the previous section and in the appendix.

5.4.3. RCRA Risk/Cost Policy Model (WET Model)

The RCRA risk/cost policy model establishes a system that allows users to investigate how trade-offs of costs and risks can be made among wastes, environments, and technologies (W-E-Ts) in order to arrive at feasible regulatory alternatives. The model was developed for EPA by ICF, Inc.

There are many components in the system. Eighty-three hazardous waste streams are ranked on the basis of the inherent hazard of the constituents they typically contain. The system assesses these waste streams in terms of the likelihood and severity of human exposure to their hazardous constituents and models their behavior in three media -- air, surface water, and ground water. The system also incorporates the mechanisms by which the constituents are affected by the environment, such as hydrolysis, biodegradation, and adsorption.

A second integral part of the system is the definition of environments in which the hazardous components are released. Thirteen environments including a special category for deep ocean waters are defined on the basis of population, density, hydrology, and hydrogeology. The system adjusts the exposure scores of

the waste streams' hazardous constituents to account for their varying effects in the three media in each of the environments.

The third component of the system consists of the technologies commonly used to transport, treat, and dispose of the hazardous waste streams. This includes 3 types of transportation, 21 treatment technologies, and 9 disposal technologies. The system determines costs and release rates for each of these technologies based on the model's existing data base. It also incorporates estimates of capacities of the technologies, the amount of waste to be disposed of, and the proximity of the wastes to the available hazardous waste management facilities.

EPA's purpose in developing the RCRA risk/cost policy model is to assist policy makers in identifying cost-effective options that minimize risks to health and the environment. The framework of the system is intended as a screen -- to identify situations that are of special concern because of the risks they pose and to determine where additional controls may not be warranted in light of the high costs involved. The framework uses a data base that is too imprecise and general to be the sole basis for regulations. The results of the model will be used in more detailed regulatory impact analysis to determine whether some type of regulatory action is warranted.

Contaminant transport is not simulated in the WET model. Rather, a ground-water exposure/risk score is tallied based on key flow and transport parameters such as hydraulic conductivity, depth to ground water, adsorption, and hydrolysis.

5.4.4. The Liner Location Risk and Cost Analysis Model

The liner location risk and cost analysis model, developed for EPA by ICF, Inc., links a risk and a cost model. The risk model simulates the chronic risk

to human health from land disposal facilities (landfills and surface impoundments) with different design technology, location, and waste stream combinations. It integrates a series of submodels and algorithms that trace constituent releases from landfills and surface impoundments to their movement through the air and ground, then to resulting human exposures, and finally to the resultant human risk. To do so, model components predict:

- Releases to ground water and subsurface transport. A failure and release submodel estimates facility failure and the quantity of leachate released; an unsaturated zone algorithm calculates the time required for the leachate to reach an underlying aquifer; and a saturated zone submodel calculates the time and concentrations of constituents reaching a downgradient well.
- Releases to air and atmospheric transport. A volatilization algorithm calculates the quantity of constituents that volatilize over time; an atmospheric transport algorithm calculates the concentrations of these constituents at the exposure points.
- Human exposure. An exposure algorithm calculates the exposure from drinking water and from breathing constituents in air.
- Health risks. A hazard estimation submodel calculates expected cancer and noncancer risks from the exposures.

The model calculates risk over a 400-year time horizon. In doing so, it embodies many assumptions: facilities operate for 20 years with a 30-year post-closure period; contamination goes undetected and uncorrected; multiple contaminants do not interact; and few constituents degrade over time, with degradation beginning only after facility failure. The model also assumes that aquifers are homogeneous and isotropic.

The companion cost model estimates the costs of land disposal facilities with differing technologies and sizes. The results of the risk model combined with the cost data from the cost model provided EPA with the capability to perform cost/risk and cost-effectiveness analysis.

The liner location model uses the TRANS model (Random-Walk Particle Transport Model) to model contaminant transport in the saturated zone. The TRANS model is discussed in the previous section and in the appendix.

5.4.5. Landfill Ban Model

The landfill ban model is a quantitative modeling procedure used by EPA to evaluate potential impacts on ground water and establish screening levels for this medium. The ground-water screening procedure involves a back calculation from a point of potential exposure at a specified distance directly downgradient from a point of release from a land disposal unit using a fate and transport model. The ground water back calculation procedure involves the application of three model components: 1) the HELP model which addresses performance of engineer controls; 2) the fate and transport model (EPASMOD) which models the behavior of constituents in the ground-water environment; and 3) the MINTEQ model which models the behavior of metals in the ground-water environment.

The HELP model was developed by EPA specifically to facilitate estimation of the amount of runoff, drainage, and leachate that may be expected to result from a hazardous waste landfill. The model predicts the water balance by performing a mass balance between flow into various components of a landfill and water leaving these components. The model uses climatology, soil, and design data to produce daily estimates of water movement across, into, through, and out of landfills.

The EPASMOD model predicts the fate and transport of constituents in the ground water. EPSMOD is a three-dimensional, steady-state, advective dispersive model which utilizes analytical solution procedures to predict transport through homogeneous and isotropic porous media. The model accounts for advection; hydrodynamic dispersion in the longitudinal, lateral, and vertical dimensions; absorption; and chemical degradation.

Estimates of metal species distributions are determined using the geochemical model MINTEQ. MINTEQ is an equilibrium model that uses the equilibrium constant approach in solving the chemical equilibrium problem.

The contaminant transport model EPASMOD is not included in the appendix of this report because it is still in the development stages and at this time is not well documented.

6. MODEL SELECTION EXAMPLE PROBLEMS

Two site-specific example problems are provided below to demonstrate the procedure for selecting the appropriate mathematical model for a particular application. The first example is an application where the objective is to perform a screening study, while the objective of the second example is to perform a detailed study. The discussions of the example problems are presented in the order that should be followed when conducting a ground-water flow and contaminant transport modeling study, with model selection being one element of the process.

6.1. SCREENING ANALYSIS EXAMPLE PROBLEM

Over 300 landfills are licensed to operate within a particular state. The state is interested in determining whether significant ground-water contamination is occurring at the sites. As a first step, the state is interested in using models to define the scope of the problem to determine if detailed investigations of several of the sites are required. At this stage, the state is not interested in detailed, site-specific assessments.

6.1.1. Objectives of the Study

The objectives of the study are to develop a generic model of the ground-water flow and contaminant transport system beneath a landfill and to perform a sensitivity analysis to determine the likelihood that a significant contamination problem might exist. The data used in the sensitivity analysis are generic values representative of the actual landfills. The sensitivity analysis consists of several model simulations using both average and conservative values for the model parameters.

The study is primarily concerned with a contaminant transport analysis of five contaminants commonly found in landfill leachates. The contaminant data have been obtained from existing data for representative sites.

6.1.2. Conceptual Model of the Study Area

Of the 300 sites in the state, 30 are chosen as a representative sample. The existing data for the 30 sites are used to develop a generic conceptual model of a typical landfill site.

For this example, we will assume the conceptual model has been developed and is very simple. It consists of a contaminant source (either point, line, or areal) at the water table beneath the landfill; a single layer, homogeneous, porous-media aquifer; and a discharge location at a specified distance downgradient. The source strengths, ground-water velocities (hydraulic conductivity and gradient), distance to the discharge, and other pertinent model inputs have been determined from the existing data for the initial simulation.

We will also assume the five contaminants of interest and their transport properties have been identified from the existing data. Dispersion, adsorption, and degradation are important processes that need to be simulated in the initial model run and adjusted in the sensitivity analysis.

6.1.3. Model Selection Process

Having developed the conceptual model, the analyst should now follow the technical criteria to determine which model or suite of models will be appropriate for this application. Because the objective of this study is to perform a generic or screening analysis, a screening model should be selected. Using a screening model allows for making several sensitivity runs relatively quickly and at low cost. Typically, such a screening model is an analytical solution, an analytical model, or a simple numerical model.

For this study, there is no point in using a detailed model since the data are not site-specific and the objective is not to predict site-specific exposure levels but rather to compare cases in a sensitivity analysis.

Since the objective is to study the transport of 5 contaminants, a contaminant transport model should be selected. The ground-water flow is not simulated in the transport model, but rather it is specified by the available data (in terms of ground-water velocity, or hydraulic conductivity and hydraulic gradient which can be used to solve for velocity). Even though ground-water flow is not simulated, the flow parameters can still be adjusted in the sensitivity analysis.

The first part of the technical selection criteria (Figure 5-1) relates to ground-water flow. Based on the conceptualization, the flow portion of the transport model should have the capability to simulate the following conditions: water table aquifer, porous media, steady state, single phase, single layer of constant thickness, and homogeneous hydraulic properties. In a contaminant transport model, all of these properties are usually represented as a uniform velocity down a one-dimensional flow path.

The second part of the technical selection criteria relates to contaminant transport. Based on the conceptualization, the transport model should have the capability to simulate the following conditions: areal source (point or line source would be sufficient), constant source term, dispersion, adsorption, and degradation. The transport can be simulated in either one, two, or three dimensions. A one-dimensional simulation is most practical since the flow is one-dimensional. However, a three-dimensional transport simulation could take

full advantage of the contaminant concentration reduction resulting from dispersion in three directions. Density effects are not important in this application.

At this point, the analyst should go to the model selection worksheet and select a transport model which has all the capabilities discussed above. Some logical choices of models are AT123D, CHAIN, or MMT. Most numerical models are too sophisticated for this application. The final selection of a single model should be based on the implementation criteria (code has been verified and documented) and on the analyst's familiarity with and access to the model.

6.2. DETAILED ANALYSIS EXAMPLE PROBLEM

6.2.1. Statement of the Problem

Benzene was disposed of in surface lagoons at an industrial site from 1960 to 1980. The disposal operation was shut down when benzene was found in residential wells downgradient (south) of the site. A network of monitoring wells sampled in 1985 show that the benzene had migrated up to a mile downgradient, was found near the surface just south of the site, was found at depth further south of the site, and concentrations ranged between 0 and 2,000 ppb.

6.2.2. Objectives of the Study

The objectives of the study were to select a ground-water flow and contaminant transport model of the site and use the model to:

1. determine the likelihood that the shallow and deep plumes are connected, and if so, identify the reason(s) for the plume to migrate to a deeper depth;

2. predict the future extent of the plume and determine if the water supply wells for a city south of the site will become contaminated; and
3. if benzene levels in the city wells could become too high, design a pump-and-treat system to cleanup/contain the plume.

6.2.3. Conceptual Model of the Study Area

The site is located in a narrow alluvial valley about 1 mile north of a small town (Figure 6-1). The waste lagoons are situated just above the water table of the regional alluvial aquifer. The aquifer consists of uniform sands and gravels over its entire depth, and its saturated thickness ranges from 0 ft along the edges at the bedrock outcrops to 100 ft in the center of the valley. The bottom of the aquifer is defined by bedrock. South of the lagoons in the area where the benzene plume appears to migrate to a lower depth, a creek cuts across the valley from east to west. Five pump tests over the study region yielded values of hydraulic conductivity that ranged between 110 ft/day and 340 ft/day. Recharge in the area is estimated as 10 in./yr and is uniformly distributed over the study area. Water levels in the valley fluctuate very little throughout the year. The only significant pumping in the area is the pumping of the city wells. The creek is located in a low-permeability zone where it cuts across the valley. A single pump test in the material yielded a hydraulic conductivity of 25 ft/day and geologic logs show that the zone is about 50-ft deep and 500-ft wide. The creek is not hydraulically connected to the aquifer.

The principal contaminant of concern is benzene. Monitoring data show the plume has migrated about 1 mile south of the site, is shallow (between 0 and 30 ft below the water table) just south of the site and north of the creek, and is deep (between 50 and 80 ft below the water table) south of the creek. The plume

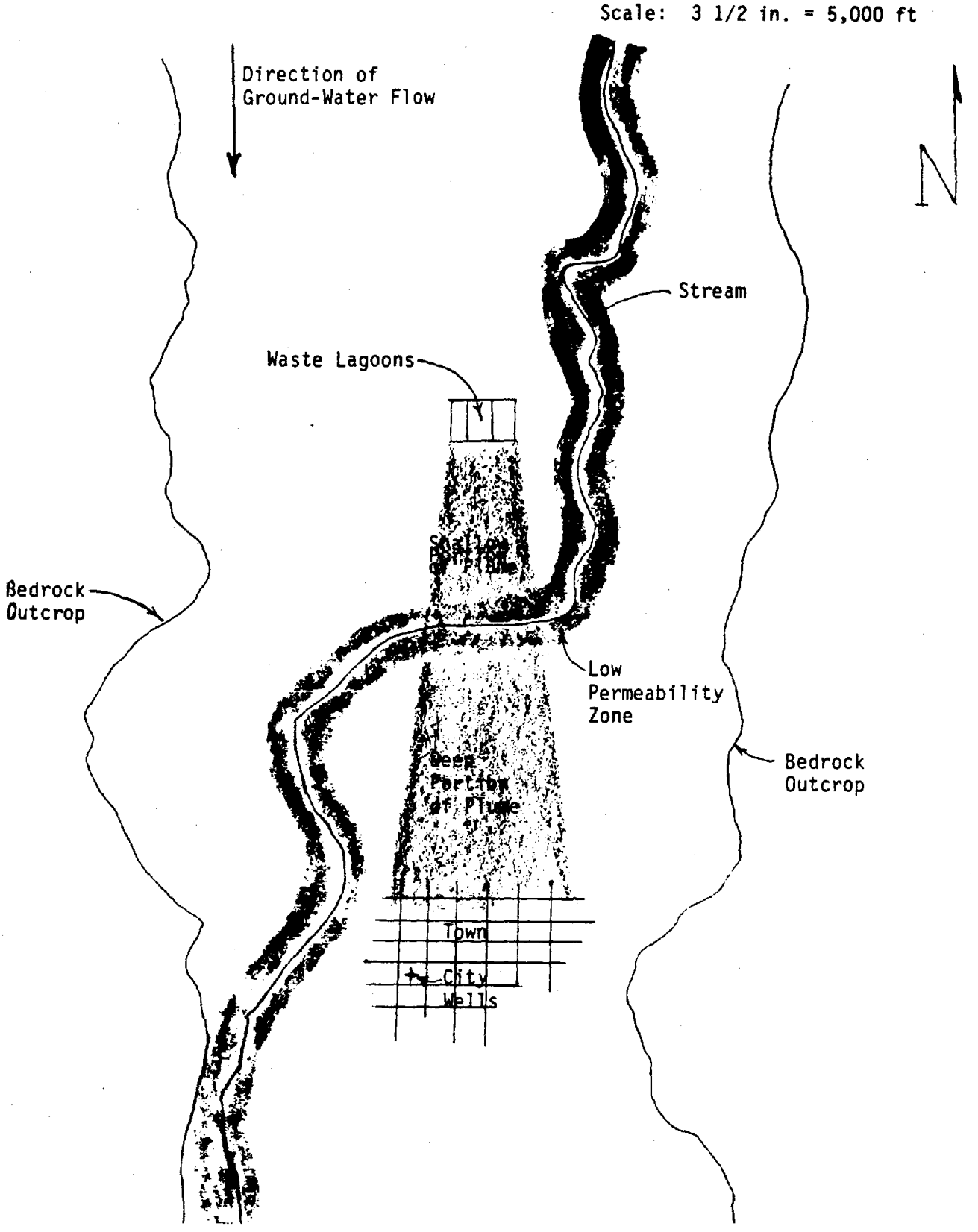

Figure 6-1. Model region for the assessment-level example problem.

has a peak concentration of about 2,000 ppb just south of the lagoons and a peak of about 100 ppb south of the creek. The width of the plume appears to be between 1,000 and 1,500 ft.

6.2.4. Model Selection Process

The model selection process first focuses on the capabilities of the ground-water flow model and then on the capabilities of the contaminant transport model. In some instances it may be possible to simulate the flow with one model and the transport with another. This is often done when using analytical solutions or simple numerical models. In more complicated, higher-dimensional problems, a single combined model is typically used.

When selecting a model based on the various criteria, the analyst can always step up to the next level but should never step back. For example, if a problem only requires a model that can simulate a single layer, the analyst can always use a model that is capable of simulating multiple layers and only simulate one.

The conceptualization of this example problem indicates that a water table model should be used. However, the water table only experiences minor fluctuations so a confined model could be used. Also, because the water table remains fairly constant, a steady-state model would be acceptable.

The flow is single phase (since benzene is soluble in water) through a porous medium. The flow occurs within a single aquifer with varying thickness. Based on the above, a porous media model that has the capability to simulate single phase flow and a single aquifer with variable thickness should be chosen.

For this problem, a three-dimensional flow model is required as a result of the partially-penetrating, low-permeability zone in the vicinity of the creek. Since the aquifer appears to be fairly homogeneous, it can be simulated with a

single value of hydraulic conductivity and porosity. However, since the low permeability zone exists along the creek, a model that allows for an areal distribution of hydraulic conductivities should be selected. Also, the model needs to allow for a vertical variation in hydraulic conductivity since the low permeability zone is only partially penetrating.

At this point the analyst can either choose a three-dimensional ground-water flow model that satisfies all the requirements (or exceeds the requirements) and select a separate transport model later, or he/she can continue with the decision process to select a coupled ground-water flow and contaminant transport model. Probably the best approach is to determine the transport model requirements before selecting any models.

Benzene entered the ground water over a period of 20 yrs (1960-1980) by leaching through the bottom of surface lagoons as it was being disposed of. Although disposal stopped in 1980, residual levels of benzene in the soils beneath the lagoons continued to leach into the ground water at reduced rates. The length of time required to leach all the benzene from the soil was estimated based on residual levels, solubility, and recharge rate. A complete sample of all monitoring wells was completed in 1985 to provide data with which to calibrate the model.

In order to calibrate the model, the analyst would simulate 20 yrs of leaching at full strength followed by 5 yrs of leaching at a reduced rate and compare the 1985 model-predicted benzene concentrations to the observed values. In order to properly simulate the release of benzene over the calibration period, the analyst needs to select a model that can simulate variable leaching rates.

To predict future concentrations, the analyst can either run the calibrated model into the future or he can run an initial value problem where the measured concentration distribution is input to the model in 1985 and the model is run into the future. For this type of a simulation, the analyst needs to select a model that can simulate an initial value problem.

The conceptual model indicates that the plume appears to migrate to a lower depth in the vicinity of the creek. In order to simulate this migration, the contaminant transport would need to be simulated in either two dimensions in the x-z plane or in three dimensions. A two-dimensional x-z model may be capable of assessing whether the plumes are connected and predicting the future extent of the plume. However, it would not be capable of aiding in the design of a pump-and-treat remedial action. A fully three-dimensional model would be required to determine well placement in the x-y plane, number of wells to pump, pumping rates, and well penetration depths.

Since benzene in this situation does not significantly degrade, a model that simulates degradation is not required.

Since there are no significant thermal or concentration gradients in the study area, density effects can be neglected. Therefore, a fully-coupled model would not be required.

At this point the analyst is ready to select a flow-and-transport model. Since the problem is fairly complex, requiring three dimensions for both flow and transport, a single combined flow-and-transport model would be the logical choice. The analyst would go to the model selection worksheet and select a flow and transport model which has all the capabilities discussed above. Some logical choices of models would be SEGOL, TRUST, GROVE/GALERKIN, PINDER, CFEST, or SWIP2. The final selection of a single model would be based on the

implementation criteria (has the model been verified and documented?) and on the analyst's familiarity with and access to the model.

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APPENDIX A

ANALYTICAL AND NUMERICAL MODEL SUMMARIES

CONTENTS

CONTENTS (continued)

ANALYTICAL FLOW

CODE NAME: PATHS

PHYSICAL PROCESSES: Analytical flow solution with pathline and travel time post processors.

DIMENSIONALITY: Two-dimensional.

SOLUTION TECHNIQUE: Analytic.

DESCRIPTION: PATHS provides an approximate contaminant transport evaluation by a direct solution of the pathline equations. The steady cases are evaluated by holding the uniform gradient, the head in the pond, and the well strengths constant. Under such steady-state conditions, only one set of flow paths, advancing fronts, and travel times must be calculated. In the transient cases, each new set of fluid particles leaving the pond or wells encounters changing velocity effects. Therefore, a range of typical departure times is selected and the flow paths, front configurations, and travel times are calculated successively for each selected set of fluid particles leaving the contaminant source. The approximate equilibrium coefficient approach is used to give the ion exchange delay effects for a single constituent. There are, however, no dispersion effects considered in the preliminary model. The model can consider as many as 35 wells at optional locations. Wells are represented asnumerically solved by the code to give the paths of the fluid particles and their advance with time toward the outflow boundary.

The LOCQUAR component completes the unit outflow rates (i.e., the water outflow volume per unit time per unit distance, along the outflow boundary). The unit outflow rate is a function of location as well as time.

The main assumptions of the code are:

- two-dimensional (horizontal plane) infinite aquifer of constant thickness;
- confined flow;
- homogeneous, isotropic material with constant properties;
- uniform flow direction may include transient gradient (flow) strength;
- round, fully penetrating wells and caverns;
- dissipation of the well and cavern heads occurs over a specified radial distance;
- diffusion and dispersion processes are neglected; and
- contaminant adsorption is based on linear equilibrium isotherms.

CODE INPUT: An interactive computer program actually coaches the user through preparation of the input file for PATHS. A worksheet is given as Table 1 in Nelson and Schur and its use is recommended because it will help ensure the use of consistent units. The interactive program can also be followed without the aid of a worksheet.

In general the PATHS code requires the following data:

- stratum thickness;
- physical properties of wells including location, radius, and flow rate;
- radial distance to remote boundary;
- x-coordinate termination of path lines;
- source radius;
- steady-state or dynamic head at source;
- hydraulic conductivity;
- effective porosity;
- uniform gradient;
- starting times and locations of pathlines;
- instructions for plots to be generated; and
- linear distribution coefficient.

CODE OUTPUT: A variety of outputs are generated by the three components of the code. There are:

1) PATHS -- Input data file for GROUND.

2) GROUND -- Hard copy lists and plots of

   - the fluid or contaminant flow paths;
   - the rate of advance and shape of the contaminant fronts moving through the system; and
   - the location and time of contaminant arrival at the outflow boundary.

3) LOCQUAR -- The water outflow volume per unit time along the outflow boundary.

COMPILATION REQUIREMENTS: The code is written entirely in FORTRAN-77. Current versions, originally developed on a Univac 1100/44 system, have been converted to a Digital Equipment Corporation VAX 11/780 systems. Some minor changes were made because the two systems differ in their file operations.

The code can capture information on 55 time planes for up to 50 pathlines and 35 wells. The wells are at arbitrary locations and are represented as completely penetrating, vertical line sources with steady or time-dependent flow rates.

PATHS is constructed in a modular fashion and appear to be easily modified. Versions exist on two hardware configurations. The software allows someone

with limited computer background to run the code. The interrogative building of the input data file coupled with the batch processing of the solution is a user-friendly and computationally efficient method.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: As an analytical solution, the validation is simply required to test for errors in formulation of the solution or in the computer coding. The results of PATHS have been compared to the results from both VTT and FE3DGW.

The PATHS model was designed to provide a balance between the refinement of the model and the limited data usually available for initial evaluation of subsurface contamination problems. It allows the user to make "first cut" evaluations inexpensively and quickly. Specific applications include:

- Initial model for movement from deep underground caverns for the Advanced Technology Development Section, Research and Engineering Department, Atlantic Richfield Hanford Company.
- Initial model of accidental release from a fuels reprocessing facility in South Carolina.
- Initial evaluation of accidental failure of earthen sewage holding ponds, Kennewick, Washington.
- Initial evaluation of seepage from a copper tailings reservoir.
- Model used in "Groundwater Engineering Short Course," sponsored by Agricultural Research Service, Chickasha, Oklahoma.
- Example evaluation for State of Idaho Department of Water Administration.
- Evaluation of a numerical generation scheme for pathlines for Atlantic Richfield Hanford Company in cooperation with the Pacific Northwest Laboratory for the U.S. Energy Research and Development Administration.
- Evaluation of potential hazard from subsurface reactor accidental releases for Sandia National Laboratories, Albuquerque, New Mexico.

DOCUMENTATION/REFERENCES:

Nelson, R.W.; Schur, J.S. (1980) PATHS -- groundwater hydraulic assessment of effectiveness of geologic isolation systems. PNL-3162, Pacific Northwest Laboratory, Richland, WA.

SOURCE: PATHS was written by R. W. Nelson and J. A. Schur and was a direct result of research conducted by Pacific Northwest Laboratory. The research was supported by the Waste Isolation Safety Assessment Program (WISAP).

ANALYTICAL TRANSPORT

CODE NAME: AT123D (Analytical Transient 1-, 2-, or 3-Dimensional)

PHYSICAL PROCESSES: Provides analytic or Green's Function solutions to the solute transport equation in 1, 2, or 3 dimensions with a constant uniform water velocity.

DIMENSIONALITY: One-, two-, or three-dimensional.

SOLUTION TECHNIQUE: Analytic.

DESCRIPTION: The code is limited to a single component, constant, uniform parallel velocity field, rectangularly shaped sources and regions of interest, with releases at a constant rate. The source may be a point, line segment, rectangle, or rectangular prism. The release may be instantaneous, continue for a finite time period (band release), or be a step function. Equilibrium adsorption and radioactive decay are included; but decay chains are not treated. Aquifers may have finite or infinite depth and width. The program output is the radionuclide concentration in the groundwater. AT123D requires that the water flow be known and be approximated by a uniform parallel flow.

The principal simplifying assumptions are as follows:

- validity of the solute transport equation;
- all boundaries are of the no-flow type;
- a constant, uniform parallel flow velocity;
- the source is a rectangular prism, and the rate and duration of release are the same everywhere within the source;
- infinite solubility; and
- release of contaminant at a constant rate over some duration.

CODE INPUT: The principal inputs are as follows:

- location and dimensions of the source;
- aquifer dimensions;
- porosity;
- hydraulic conductivity;
- hydraulic gradient;
- dispersivity;
- distribution coefficient; and
- duration of release.

CODE OUTPUT: The output of the code is a series of tables showing concentration at selected points and selected times.

COMPILATION REQUIREMENTS: AT123D is written in FORTRAN IV, and should be adaptable to most computers. Current problem limits are as follows:

- 15 x-locations for output;
- 10 y-locations for output;
- 10 z-locations for output;
- 1,200 time steps; and
- 1,000 eigenvalues for series evaluation.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The code has been checked against hand calculations and laboratory experiments. The code is in the public domain.

DOCUMENTATION/REFERENCES:

Yeh, G.T. (1981) AT123D: analytical transient one-, two-, and three-dimensional simulation of waste transport in the aquifer system. ORNL-5602, Oak Ridge National Laboratory, Oak Ridge, TN.

SOURCE: AT123D was written by G. T. Yeh at Oak Ridge National Laboratory.

CODE NAME: CHAIN

PHYSICAL PROCESSES: Convective-dispersive solute transport, saturated or unsaturated steady flow, sequential first order radioactive decay, linear sorption.

DIMENSIONALITY: One dimensional.

SOLUTION TECHNIQUE: Analytical based upon LaPlace transforms.

DESCRIPTION: CHAIN presents analytical solutions to solute transport involving sequential first-order decay in saturated or unsaturated soil systems. Solutions of the simultaneous movement of up to four member chains are provided for the one-dimensional convective-dispersion equation. A degrading source term may be modeled by invoking the solution to the Bateman equations. The main assumptions of the code are:

- steady groundwater flow;
- constant pore velocity and dispersivity over path length;
- linear geochemical sorption model;
- linear decay with up to four members;
- initial value or flux source condition; and
- degrading source term.

CODE INPUT:

- path lengths;
- pore velocity;
- water content;
- dispersivity;
- decay constants;
- retardation coefficients; and
- time for which solute concentration are calculated.

CODE OUTPUT: Solute concentrations at various times and positions along path for up to four members of chain.

COMPILATION REQUIREMENTS: CHAIN is written in FORTRAN and may be easily installed on essentially all computer systems.

EXPERIENCE REQUIREMENTS: Moderate.

TIME REQUIREMENTS: Days.

CODE VERIFICATION: Numerous numerical verification problems are provided in the user's manual which has been published in the open literature. Field validation has been performed for the convective-dispersion equation in numerous tracer experiments in the saturated and unsaturated zones.

DOCUMENTATION/REFERENCES: A full user's manual and documentation may be found in

VanGenuchten, M.Th. (1985) Convective-dispersive transport of solutes involved in sequential first-order decay reactions. Con. of Geosciences 2:129-147.

SOURCE: M. Th. VanGenuchten
U.S. Salinity Laboratory
4500 Glenwood Drive
Riverside, CA 92501

CODE NAME: GETOUT

PHYSICAL PROCESSES: Predicts the transport of radionuclide chains along a one-dimensional path.

DIMENSIONALITY: One dimensional.

SOLUTION TECHNIQUE: Analytical.

DESCRIPTION: The model interfaces directly with the water-dose models, ARRG and FOOD, and together they are used to predict the dose consequences to people from radionuclide releases.

The model analyzes the transport of radionuclides by flowing groundwater following a leach incident at an underground nuclear waste disposal site. This model assumes that at some arbitrary time after the waste is deposited, the contents of the site are dissolved at a specific constant rate by groundwater. The groundwater flows at constant velocity through a homogeneous one-dimensional column of the geologic medium and discharges to a surface water body. The dissolved radionuclides are assumed to be in sorption equilibrium at all points in the geologic medium. Radioactive decay (including chain decay of the actinides) is modeled both at the disposal site and during migration through the geologic medium. Trace concentrations of the dissolved nuclides are assumed and, as a result, the adsorption equilibrium constants are independent of concentrations. A constant axial dispersion coefficient is also assumed. This model is applicable to particulate and fractured media, provided the necessary input data are obtained properly and it can be applied to heterogeneous media if a weighted averaging technique is properly applied to the relevant input parameters.

CODE INPUT: Inputs for GETOUT include:

- time leaching beings;
- duration of leaching;
- path length;
- pore velocity of water; and
- dispersion coefficient.

CODE OUTPUT: The output of the code is the rate of discharge of each nuclide. Digital and graphic output is printed and results are written to a file that can be read by the biosphere code FOOD. Peak discharge rates are reported for key nuclides.

COMPILATION REQUIREMENTS: GETOUT is written in FORTRAN IV and implemented on a UNIVAC-1100/44 EXEC-8 system. It has been converted to CDC equipment.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Verification work by E. L. J. Rosinger at Whiteshell (ref. 4) uncovered problems in early unpublished versions of the code and confirmed the accuracy of the published version by comparison with analytic solutions. The code is in the public domain.

DOCUMENTATION/REFERENCES:

DeMier, W.V.; Cloninger, M.O.; Burkholder, H.C.; Liddell, P.J. (1979) GETOUT -- a computer program for predicting radionuclide decay chain transport through geologic media. PNL-2970, Pacific Northwest Laboratories.

Burkholder, H.C.; Cloninger, M.O.; Baker, D.A.; Jansen, G. (1976) Incentives for partitioning high-level waste. Nuclear Technology 31:150, also as BNWL-1927, Pacific Northwest Laboratories Report BNWL-1927.

Lester, D.H.; Jansen, G.; Burkholder, H.C. (1975) Migration of radionuclide chains through an adsorbing medium. AIChE Symposium Series 152, Adsorption and Ion Exchange 71.

Burkholder, H.C.; Rosinger, E.L.J. (1980) Nuclear Technology 49.

Elert, M.; Grundfelt, B.; Stenquist, C. KBS Teknisk Rapport 79-18.

SOURCE: GETOUT was originally written by D. H. Lester, H. C. Burkholder, and M. O. Cloninger at Pacific Northwest Laboratory. The current FORTRAN IV version was developed by H. C. Burkholder, M. O. Cloninger, W. V. DeMier, and P. J. Liddell.

CODE NAME: GWMTM1 and GWMTM2 (Groundwater Mass Transport Model 1 Dimensional and 2 Dimensional)

PHYSICAL PROCESSES: Determines contaminant concentrations in the vicinity of a decaying source under steady-state flow conditions.

DIMENSIONALITY: One or two dimensional depending upon code used.

SOLUTION TECHNIQUE: Analytical.

DESCRIPTION: The codes are deterministic, one- or two-dimensional analytical solutions of the transient convective-dispersive mass transport equation modified for first-order decay, with an exponentially decaying, Gaussian boundary condition. The one-dimensional model is designed to solve for vertical infiltration of wastewater through saturated or unsaturated soil media under constant vertical seepage velocity. Presumably it could be used to model one-dimensional horizontal transport also under steady-state flow conditions. The two-dimensional code is designed for estimating the two-dimensional (areal or vertical cross section) concentration pattern downgradient from sanitary landfills, wastewater lagoons, or other groundwater pollution sources.

CODE INPUT: GWMTM1: Dispersion coefficient, kinetic decay constant, constant seepage velocity, and surface constant (if surface concentration is not constant), user specified space, and time positions.

GWMTM2: Fewer than ten cards for parametric information plus space and time positions for desired concentration calculations.

CODE OUTPUT: Concentrations are printed at user-specified locations in space and time.

COMPILATION REQUIREMENTS: The model is written in standard FORTRAN IV and has been run on an S/360/91; it should run on any standard digital computer. The program requires a region size of approximately 100K on the S/360/91. One can learn to run the model in less than a half hour and only four FORTRAN statements need to be punched (space and time positions are specified as data cards). Setup time is insignificant and FORTRAN programming knowledge is unnecessary. It has also been run on minicomputers using less than 100K of core.

EXPERIENCE REQUIREMENTS: Minimal.

TIME REQUIREMENTS: Days.

CODE VERIFICATION: The two-dimensional version has been "used to check the numerical accuracy of several solution schemes of two-dimensional, numerical models of groundwater quality. It has been distributed widely through short courses dealing with groundwater pollution and has been used principally to simulate leachate plumes from landfills and check the accuracy of two-dimensional, numerical models."

DOCUMENTATION/REFERENCES:

Professor Robert W. Cleary
P. O. Box 2010
Princeton, NJ 08540

Cleary, R.W. (1977) Final 208 report to the Naussau-Suffolk Regional Planning Board, Hauppauge, New York.

SOURCE: Bob Cleary, Princeton, NJ.

CODE NAME: NUTRAN

PHYSICAL PROCESSES: NUTRAN calculates the consequences (in terms of releases of radioactivity or doses to humans) of groundwater releases of radioactivity from a repository. NUTRAN evaluates the combined effect of systems of natural and engineered barriers; some barriers are modeled in detail and others are simply characterized by a number summarizing their performance (e.g., for a canister, lifetime).

DIMENSIONALITY: One, two, or three dimensional.

SOLUTION TECHNIQUE: Analytical.

DESCRIPTION: The principal phenomena treated by NUTRAN are:

- the resaturation of the repository cavity with water;
- leaching of the waste matrix;
- dissolution of the radioactive elements in the waste;
- diffusion through clay cylinders around waste canisters;
- transport of waste by groundwater through the repository, surrounding strata, and adjacent aquifers (calculated using a network of one-dimensional flow paths, with a two-dimensional method used for aquifers containing wells);
- withdrawal of contaminated groundwater through wells;
- transport of waste in surface waters and associated ecosystems; and
- human exposure and dose mechanisms.

NUTRAN performs most of the functions involved in analyzing long-term effects of a waste repository. NUTRAN contains only an extremely simple model for groundwater flow. In many cases the results of a flow code such as VTT must be used to prepare the inputs to NUTRAN. Among these cases are those in which two- or three-dimensional effects are important or thermal convection or large density gradients are present.

The code is based on representing the flow field as a network of one-dimensional path segments. Arbitrary numbers and configurations of path segments can be accommodated. Simple models of several of the engineered barriers in the repository and waste package are also included.

The principal assumptions of the code are:

- the one-dimensional solute transport equation is valid within each path segment;
- sorption may be represented as equilibrium adsorption;
- once a canister has any holes in it, it disappears entirely as a barrier to waste dissolution;

- when a clay buffer cylinder is present, wastes diffuse through it in approximately a steady state; and
- water in waste storage rooms is well mixed.

CODE INPUT: NUTRAN permits the user to divide nuclides into classes with identical sorption behavior. It also permits "states" with different water flow to occur over time. The principal inputs to WASTE are as follows:

- retardation factor of each class of nuclides in each leg in each state;
- cross-sectional area of each leg in each state;
- longitudinal dispersivity of each leg;
- hydraulic conductivity of each leg in each state;
- heads at leg junctions in each state;
- length of each leg;
- effective porosity of each leg in each state;
- repository dimensions and backfill characteristics;
- age of wastes at repository commissioning;
- canister lifetime;
- rates or times of transitions among states;
- solubilities of any nuclides (optional);
- locations and pumping rates of wells; and
- transverse dispersivity of aquifer from which wells draw.

The inputs to PLOT, other than disk files written by ORIGEN, BIODOSE, and WASTE, usually consist only of control variables.

CODE OUTPUT: The primary output of NUTRAN is the rate at which radioactivity is released or the dose to individuals or populations. Both totals due to all nuclides and the contributions of any number of individual nuclides selected by the user are available. Doses or release rates are given as functions of time with peak values identified; release rates and population doses may also be integrated over all time. Both digital and graphic output may be obtained.

A variety of intermediate quantities used in the calculations may also be output.

COMPILATION REQUIREMENTS: The code is written in PL/I and has been run on a number of IBM machines. The user must supply IMSL (International Mathematical Statistical Language) routines and, if graphical output is desired, the DISSPLA plotting package is used. The test cases in the User's Guide require 2 to 3 minutes CPU time on an IBM 370/3031. BIODOSE requires one megabyte of core;

WASTE and PLOT require 512 K. A small amount of disk storage is required for communication among the programs.

TASC has not released the program to the public.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: NUTRAN has been compared to GETOUT and BIOPATH for a one-dimensional problem (ref. 1), and to a number of analytic solutions.

DOCUMENTATION/REFERENCES:

Ross, B.; Koplik, C.M.; Giuffre, M.S.; Hodgin, S.P. (1981) A computer model of long-term hazards from waste repositories. Radioactive Waste Management 1:325-338.

Ross, B., Koplik, C.M.; Giuffre, M.S.; Hodgin, S.P.; Duffy, J.J. (1979) NUTRAN: a computer model of long-term hazards from waste repositories. The Analytic Science Corporation Report UCRL-15150.

Ross, B.; Koplik, C.M. (1979) A new numerical method for solving the solute transport equation. Water Resour. Res. 15:949-55.

Giuffre, M.S.; Ross, B. (1979) The effect of retardation factors on radionuclide migration. In G. J. McCarthy, ed., Scientific Basis for Nuclear Waste Management 1:439-442, Plenum, NY, and Longon.

Ross, B ; Koplik, C.M. (1978) A statistical approach to modeling transport of pollutants in ground water. Mathematical Geology 10:657-672.

Berman, L.E.; Ensminger, D.A.; Giuffre, M.S.; Koplik, C.M.; Oston, S.G.; Pollak, G.D.; Ross, B.I. (1978) Analysis of some nuclear waste management options. The Analytic Sciences Corporation Report UCRL-13917.

Ross, B.; Koplik, C.M.; Giuffre, M.S.; Hodgin, S.P.; Duffy, J.J.; Nalbandian, J.Y. (1980) User's guide to NUTRAN: a computer analysis system for long-term repository safety. Atomic Energy of Canada, Ltd., Technical Report AECL-TR-121.

SOURCE: The code was developed by B. Ross, C. M. Koplik, M. S. Giuffre, J. J. Duffy, S. P. Hodgin, and others at the Analytic Sciences Corporation.

CODE NAME: NWFT/DVM (Network Flow and Transport/ Distributed Velocity Method)

PHYSICAL PROCESSES: Predicts fluid flow and transport of radionuclide chains. The rate at which nuclides enter groundwater can be limited by both leach rates and equilibrium solubility. Water velocities can reflect density forces caused by nonuniformities in salt concentrations.

DIMENSIONALITY: One dimensional.

SOLUTION TECHNIQUE: Numerical convolution of analytical solution for a discretized flow network; utilizes the "distributed velocity method."

DESCRIPTION: NWFT/DVM uses a network of one-dimensional flow paths. A steady-state water velocity is calculated in each path, with pressures and brine densities considered. Radionuclides enter groundwater at a rate determined by the combined effects of kinetic leaching and equilibrium solubility. Transport of radionuclides can be handled by either an analytic solution (similar to GETOUT and NUTRAN) within each path segment (or "leg") or by the Distributed Velocity Method (DVM) which is unique to this code. Daughter nuclides whose velocity differs from their parents' must be treated by DVM.

NWFT/DVM is a far-field code. It is designed to analyze repositories in well stratified sedimentary rocks. NWFT/DVM is finite-difference or finite-element code.

The principal assumptions of the code are:

- fluid flow proceeds only along a specified network of 15 path segments;
- Darcy's Law is valid;
- the one-dimensional solute transport equation is valid within each path segment;
- thermal convection can be neglected;
- all water flowing through the repository contacts the waste;
- brine concentration and pressures do not change over time; and
- sorption can be represented as equilibrium adsorption.

CODE INPUT: Inputs for NWFT/DVM include:

- conductivity in each leg;
- cross-sectional area of each leg;
- elevation of each node;
- porosity of each leg;
- rock density in each leg (optional);

- brine concentration in each leg;
- mass of each nuclide;
- half life of each nuclide;
- initial inventory of each nuclide;
- distribution coefficient of each nuclide in each leg;
- leach time;
- dispersion constant (same value everywhere);
- solubility of each nuclide;
- time leaching beginnings; and
- cutoff time.

CODE OUTPUT: The principal output is the discharge rate of each nuclide in Ci/day as a function of time. The total integrated discharge and the peak discharge rate are also given. A variety of intermediate quantities can be output as well.

COMPILATION REQUIREMENTS: The code is written in FORTRAN. The code uses one IMSL (International Mathematical Statistical Library) routine to solve a system of linear equations. This routine or a substitute must be supplied by the user.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Results from NWFT/DVM have been compared with results of GETOUT for a range of one-path-segment problems. Also, it has been compared to SWIFT for a problem with a six-member decay chain. The code is in the public domain.

DOCUMENTATION/REFERENCES:

Campbell, J.E.; Longsine, D.E.; Cranwell, R.M. (1981) Risk methodology for geologic disposal of radioactive waste: the NWFT/DVM computer code user's manual. Sandia National Laboratories Report NUREG/CR-2081.

NWFT/DVM lecture notes. Draft, Sandia National Laboratories.

Campbell, J.E.; Longsine, D.E.; Reeves, M. (to be published) The distributed velocity method of solving the convective-dispersion equation.

SOURCE: The NWFT/DVM model was developed at Sandia National Laboratories. The original NWFT model was developed at Sandia and INTERA Environmental Consultants by Campbell, Kaestner, Langkopf, and Canty. NWFT/DVM incorporates the DVM, developed by Campbell and Longsine of Sandia and Reeves of INTERA.

NUMERICAL FLOW (SATURATED/UNSATURATED)

CODE NAME: FEMWATER1

PHYSICAL PROCESSES: Predicts groundwater flow through saturated or unsaturated porous media.

DIMENSIONALITY: Two dimensional (x-y, x-z cartesian).

SOLUTION TECHNIQUE: Numerical, finite element, quadrilateral element.

DESCRIPTION: FEMWATER1 is a revision of the Yeh and Ward subsurface flow model. It is a flow-only code that creates a data file specifically for the operation of the FEMWASTE1 pollutant transport model. FEMWATER1 applies to flow in porous media which is:

- transient or steady state;
- two dimensional (horizontal or vertical cross section); and
- saturated-unsaturated.

The model is based on the conservation of mass and momentum and includes soil and water compressibility effects. Water is exchanged between the surface and subsurface media by:

- seepage or ponding;
- infiltrating runoff from rainfall;
- artificial recharge and withdrawal; and
- ponds, lakes, and streams.

FEMWATER1 uses quadrilateral bilinear and triangular finite elements to represent the two-dimensional porous media domain. The Galerkin method of weighted residuals is used to solve the continuity equation and Richards' equation. Finite difference discretization of the time derivatives can be specified in one of three ways:

1) backward difference;

2) central difference; or

3) mid-difference.

The mid-difference time stepping scheme was added to the previously available options of central and backward differencing schemes. The method of mid-differencing assumes linear variation of the unknown variable over the time interval such that the computer matrices are evaluated at the midpoint of the time interval.

With the three time stepping and two mass lumping options, six numerical solution procedures are available in FEMWATER1. Other than the general recommendations above, no discussion of the stability or accuracy characteristics of the various solutions is presented.

Soil properties and hydraulic conductivities in FEMWATER1 are functions of pressure head alone. Because pressure head is the dependent variable, the equation set to be solved is nonlinear, requiring iterative solution techniques. The Newton-Raphson iteration with the option of over- and under-relaxation is used. For large problems, a line successive over-relaxation technique is available.

Unlike most flow models that calculate the velocity field by taking derivatives of the solved pressure field, FEMWATER1 formulates Darcy's Law with the finite element solution method. This approach has the advantage of continuous velocity distributions at the model boundaries.

Mass balance computations are built into FEMWATER1 to monitor numerical error generation.

The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow; and
- the nonlinear soil properties and the hydraulic conductivity are functions of the pressure head only.

CODE INPUT: Inputs to FEMWATER1 include:

- grid geometry;
- initial heads;
- prescribed head and flux boundary conditions;
- hydraulic-conductivity tensor;
- modified storage coefficient; and
- material nonlinearities.

CODE OUTPUT: The output from FEMWATER1 consists of the pressure distribution and velocity field at each time step.

COMPILATION REQUIREMENTS: FEMWATER1 is written in FORTRAN and was originally installed on an IBM 360 machine. The code is generally compatible with most all mainframe or virtual memory machines.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Two sample problems to which solutions had previously been obtained by other validated numerical models, namely 1) the seepage pond problem and 2) the Freeze transient problem, were solved. In addition, results by all six alternative numerical schemes discussed below in the section on numerical approximations were compared in both examples. No field validation has been performed.

DOCUMENTATION/REFERENCES:

Yeh, G.T.; Ward, D.S. (1979) FEMWATER: a finite-element model of water flow through saturated-unsaturated porous media. Oak Ridge National Laboratory Report ORNL-5567.

Reeves, M.; Duguid, J. O. (1976) Water movement through saturated-unsaturated porous media: a finite-element Galerkin model. Oak Ridge National Laboratory Report ORNL-4927.

SOURCE: FEMWATER1 was developed at Oak Ridge National Laboratory by G. T. Yeh and D. S. Ward. It is an extension of work done by Reeves and Duguid. The code is in the public domain.

CODE NAME: FREEZE

PHYSICAL PROCESSES: Predicts water flow in a groundwater basin under transient saturated-unsaturated conditions.

DIMENSIONALITY: Three dimensional.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: A three-dimensional finite-difference model has been developed for saturated-unsaturated transient flow in small, nonhomogeneous, anisotropic geologic basins. The uniqueness of the model lies in its inclusion of the unsaturated zone in a basin-wide model that can also handle both confined and unconfined saturated aquifers under both natural and developed conditions. The integrated equation of flow is solved by the line successive overrelaxation technique. The model allows any generalized region shape and any configuration of time-variant boundary conditions. When applied to natural flow systems, the model provides quantitative hydrographs of surface infiltration, groundwater recharge, water table depth, and stream base flow.

Results of simulations for hypothetical basins provide insight into the mechanisms involved in the development of perched water tables. The unsaturated basin response is identified as the controlling factor in determining the nature of the base flow hydrograph. Application of the model to developed basins allows one to simulate not only the manner in which groundwater withdrawals are transmitted through the aquifer, but also the changes in the rates of groundwater recharge and discharge induced by the withdrawals. For any proposed pumping pattern, it is possible to predict the maximum basin yield that can be sustained by a flow system in equilibrium with the recharge-discharge characteristics of the basin.

CODE INPUT: Inputs consist of standard unsaturated or saturated zone hydrologic parameters.

CODE OUTPUT: Output consists of a pressure or head distribution.

COMPILATION REQUIREMENTS: FREEZE is written in FORTRAN and is operational on an IBM system.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Freeze, R.A. (1971) Three-dimensional transient saturated-unsaturated flow in a ground water basin. Water Resour. Res. 7(2):347-366.

SOURCE: This code was developed by R. A. Freeze of the University of British Columbia. The code is in the public domain.

CODE NAME: UNSAT1

PHYSICAL PROCESSES: Provides a simulation capability for flow in a one-dimensional unsaturated or saturated soil column.

DIMENSIONALITY: One dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The UNSAT1 model provides numerical solutions to the one-dimensional flow problem of an unsaturated-saturated medium. It employs a Galerkin finite-element analysis of this one-dimensional physical domain. The hermite cubic polynomial is used as the basis for the finite-element approximation to the continuum.

CODE INPUT: Inputs consist of standard unsaturated or saturated zone hydrologic parameters..

CODE OUTPUT: Output consists of a pressure or head distribution.

COMPILATION REQUIREMENTS: UNSAT1 is written in FORTRAN IV.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

van Genuchten, M.Th. Numerical solutions of the one-dimensional saturated-unsaturated flow equation. 78-WR-09, Princeton University, Princeton, NJ.

SOURCE: This code was written by M. Th. van Genuchten of the U.S. Salinity Laboratory. The code is in the public domain.

CODE NAME: UNSAT2

PHYSICAL PROCESSES: Simulates nonsteady seepage in saturated or unsaturated porous media.

DIMENSIONALITY: Two dimensional (x-y or x-z cartesian). Axisymmetric (r-z cylindrical).

SOLUTION TECHNIQUE: Numerical, finite element, triangular elements.

DESCRIPTION: The program can be used to investigate problems involving two spatial dimensions in the horizontal or vertical plane. Three-dimensional problems can be handled provided that the flow pattern retains an axial symmetry about the vertical coordinate. The flow region may have any complex shape and it may consist of different soil materials arranged in arbitrary patterns. Each soil material may exhibit an arbitrary degree of local anisotropy with the principal hydraulic conductivities oriented at any desired angle with respect to the coordinates.

A wide range of time-dependent boundary conditions can be treated: prescribed pressure head; prescribed flux normal to the boundary; seepage faces and evaporation and infiltration boundaries where the maximum rate of flux is prescribed by atmospheric or other external conditions while the actual rate is initially unknown. In addition, the program can handle water uptake by plants assuming that the maximum rate of transpiration is determined by atmospheric conditions while the actual rate of uptake depends on atmospheric as well as soil and plant conditions. Internal volumetric sinks or sources of prescribed strength can be included in the flow system at any stage of the computation. A special provision has been made for the analysis of axisymmetric flow to a well of finite radius partially penetrating an unconfined aquifer system and discharging at a prescribed time-dependent rate. The well may be partially cased and its capacity for storing water is taken into account. Several layers can be tapped by the well at the same time.

The domain simulated by UNSAT2 is discretized using three-noded triangular elements. The time domain is discretized by finite-difference techniques.

The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow;
- the rate of uptake by roots is proportional to the pressure head gradient across the soil-root interface;
- there is no hysteresis in the water retention or relative permeability curves; and
- the relative permeability and capillary pressures are functions of moisture content.

CODE INPUT: Inputs to UNSAT2 include:

- grid geometry;

- initial heads (total head or pressure head);
- boundary conditions;
- rates of infiltration, evaporation, and transpiration;
- root effectiveness function;
- hydraulic conductivity tensor;
- relative permeability function;
- capillary pressure function; and
- storage coefficient.

CODE OUTPUT: The printed output of the program consists of a listing of all input information, a complete description of the finite-element network, the boundary codes of all nodes, and the properties of each material. During each time step the program prints a listing of total head values, pressure head values, moisture content values, and discharge into or out of the system (not flow through the system) at all nodes. The rate of convergence of the iterative procedure is printed during each time step together with additional information pertaining to the particular problem at hand.

COMPILATION REQUIREMENTS: UNSAT2 is written in FORTRAN IV and was originally installed on an IBM 370/165 machine. The code is generally compatible with most all mainframe or virtual memory machines.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Due to the lack of analytic solutions to problems of flow in the unsaturated zone at the time UNSAT2 was developed, verification could only be performed by comparing the results to results obtained from other, previously validated, numerical models. The effect of vertical flow in the presence of evapotranspiration was simulated using both a finite-difference code and the finite-element code, UNSAT2. The results were compared.

Two field problems were simulated by UNSAT2 as reported in Ref. 1. These are: 1) a field experiment performed by Feddes (ref. 2) at the groundwater level experimental field Geestmerambacht in the Netherlands, and 2) a field experiment taken from the subirrigation experimental field "De Groeve" in the Netherlands (ref. 3).

DOCUMENTATION/REFERENCES:

Neuman, S.P.; Feddes, R.A.; Bresler, E. (1974) Finite element simulation of flow in saturated-unsaturated soils considering water uptake by plants. Technion, Hydrodynamics, and Hydraulic Eng. Laboratory Report, July.

Feddes, R.A. (1971) Water, heat, and crop growth. Thesis Comm. Agric. Univ. Wageningen 71-12, pp. 184.

Feddes, R.A.; van Steenbergen, M.G. (1973) Sub-irrigation field 'De Groeve'." Mpta 735, Inst. for Land and Water Management Res., Wageningen, pp. 184.

Feddes, R.A.; Bresler, E.; Neuman, S.P. (1974) Field test of an improved numerical model for water uptake by root systems. Unpublished manuscript.

Hanks, R.J.; Klute, A.; Bresler, E. (1969) A numeric method for estimating infiltration, redistribution, drainage, and evaporation of water from soil. Water Resour. Res. 5(5):1064-1069.

Neuman, S.P. (1972b) Finite element computer programs for flow in saturated-unsaturated porous media. Second Annual Report, Project No. A10-SWC-77, Hydraulic Engineering Laboratory, Technion, Haifa, Israel, pp. 87.

Neuman, S.P. (1973) Saturated seepage by finite elements. Proc. ASCE, J. Hydraul. Division, 99(HY12):2233-2250.

SOURCE: UNSAT2 was developed at Technion, Israel Institute of Technology, by S. P. Neuman, R. A. Feddes, and E. Bresler. The code is in the public domain.

NUMERICAL FLOW (SATURATED)

CODE NAME: BEWTA

PHYSICAL PROCESSES: Predicts the Boussinseq equation for a two-dimensional water table aquifer.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite-difference.

DESCRIPTION: The aquifer is given by a two-dimensional discrete representation in the horizontal plane. Its boundary is irregular and mixed, and it is superimposed by a meandering stream. Aquifer parameters are assigned to each nodal point and an be slightly anisotropic and nonhomogeneous. Transient groundwater flow through a water table aquifer is described by the Boussinesq equation, which assumes that the Dupuit-Forchheimer assumptions are valid. The principal conductivity components are colinear with the coordinate system X and Y. The water is released from storage mainly by gravity drainage with an instantaneous decline in head. The stream bed is semi-confined, and the leakage obeys Darcy's Law. The flow from the unsaturated zone and the change in fluid density over time are negligible. Replenishment of the aquifer system occurs through gravity drainage and stream bed leakage.

The model simulates transient groundwater flow through a two-dimensional water table aquifer using the alternative direction implicit method. The Boussinesq equation is approximated by a two-dimensional finite-difference equation of linearized form, employing the noniterative alternating direction implicit method. The equation is written for two half-time steps, and is done for each node along either a row or a column. The resulting simultaneous equations are solved by the Thomas algorithm. The calculations are carried on successionally row by row for the first half-time step and column by column for the second half-time step (where results are approximations to the transient solution of the problem under discussion).

CODE INPUT: Standard saturated zone hydrologic parameters.

CODE OUTPUT: Head distribution at each time step.

COMPILATION REQUIREMENTS: BEWTA is written in FORTRAN.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES: Not available.

SOURCE: BEWTA was developed by Chang L. Lin of the Nova Scotia Department of the Environment.

CODE NAME: COOLEY

PHYSICAL PROCESSES: Predicts the transient or steady-state hydraulic head distribution and velocity flow field in a confined, semiconfined, or unconfined aquifer.

DIMENSIONALITY: Two-dimensional (x-y or x-z cartesian, r-z radial).

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The code is applicable to confined, semiconfined, or unconfined flow problems which obey the generalized Boussinesq equation. Flow may be steady or nonsteady. The aquifer may be given an areal (plan view) or radial description or may be cross sectional. Aquifer parameters may be distributed or zoned and the system may be anisotropic with the principal components aligned with the global coordinate axes. In the areal description, if used, leakage from confining beds (or river bottoms, etc.) is vertical and storage in the confining beds is neglected. The Dupuit-Forchheimer assumptions and delayed (or no delayed) yield constant are used for the water table case in plan view. The basic discretization method is the subdomain finite-element method with the time discretized by a weighted average technique.

COOLEY is best suited for a single layer aquifer system. A layered aquifer system, however, may be analyzed within using the radial coordinate system. The code represents a two-dimensional area, whether areal, plane cross sectional, or axisymmetric cross sectional, as a series of zones. The zone shapes may be triangular or quadrilateral and of nearly any convex shape except that the boundaries must pass through, and not between, all nodes.

There are three basic versions of the program, the differences among them being the methods used to solve the matrix equation. The choice depends on the site.

COOLEY is most applicable to porous media. Fractured media can also be modeled if the fractures are sufficiently numerous that they can be approximated by a porous medium.

The principal numerical approximations in COOLEY are the following:

- Discretization of space by the finite-element method of using the "subdomain collocation" version of the weighted residual method (ref. 3, p.40).
- Discretization of time by the explicit Euler forward difference, the semi-implicit Crank-Nicholson central difference, or the fully implicit backward difference scheme.

The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanisms for fluid flow.
- The porosity and hydraulic conductivity of the aquifer are constant with time.

- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- Assumptions analogous to the Dupuit-Forchheimer assumptions are used for unconfined aquifers.
- The transmissivity tensor has principal axes parallel to the coordinate axes.

CODE INPUT: Inputs to COOLEY include:

- grid geometry;
- prescribed head and flux boundary conditions;
- transmissivity in both x and y (or r and z) directions;
- storage coefficient or specific yield for areal problems and specific storage for cross-sectional or radial-flow problems;
- hydraulic conductance for an adjacent aquitard for areal flow problems;
- known recharge or discharge rates; and
- initial hydraulic-head distribution.

CODE OUTPUT: The output from COOLEY consists of the pressure distribution and velocity field at each time step.

COMPILATION REQUIREMENTS: The basic programs are dimensioned such that the maximum mesh size is 50 by 50 (2500) nodes, and the maximum number of time steps is 100. In addition, the maximum number of iterations for program LSOR is 100. With these dimensions, LSOR and ADIPIT occupy about 25,000 words and SIP occupies about 32,500 words of core on a CDC 6400 computer. However, the dimensions can easily be modified to accommodate other problem sizes and smaller or larger computers. No special library functions or subroutines are used, and the only peripheral equipment needed is a card reader. The final versions of the program were tested on a CDC 64000 computer. COOLEY is programmed in FORTRAN IV.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The code was verified for four problems to which analytical solutions were available.

Field validation runs simulated the influence of seasonal pumping of irrigation wells on groundwater levels in Ash Meadows, California, and Nevada.

DOCUMENTATION/REFERENCES:

Cooley, R.L. (1974) Finite element solutions for the equations of groundwater flow. Nevada University.

Bear, J. (1972) Dynamics of fluids in porous media. New York, NY: American Elsevier.

Zienkiewicz, O.C. (1971) The finite element method of engineering science. London: McGraw-Hill.

SOURCE: COOLEY was developed at the Center for Water Resources Research, Desert Research Institute, University of Nevada, by R. L. Cooley. The code is in the public domain.

CODE NAME: FE3DGW

PHYSICAL PROCESSES: Saturated groundwater flow in a homogeneous or heterogeneous geological system. The code provides water flow paths and travel times.

DIMENSIONALITY: Three-dimensional, radial flow (r-z).

SOLUTION TECHNIQUE: Numerical, finite element quadrilateral elements.

DESCRIPTION: FE3DGW is a set of codes designed to be executed in uncoupled stages. This allows the user to verify the accuracy of the input data before a full simulation is made, while storing information on disk for access by the main program. A plotting package is included in the data preprocessing stage to display node and element locations and vertical logs of the hydrogeologic strata. Contour plots of potential surfaces and strata interfaces are produced in three-dimensional projections to help identify obvious errors. Once the model parameters have been stored successfully on disk, they need not be processed again unless the problem configuration is changed. This is because boundary conditions are entered in a separate stage of the data storage process.

The equation set is linear with spatially varying conductivities. Convergence will be perfect if the integration of the element volumes is exact. A Gaussian quadrature scheme using two, three, or five integration points is used for the numerical integration. A necessary condition for convergence is that the basis functions used in the Galerkin technique must be defined such that constant values of any of the first derivatives are available throughout the element when suitable nodal values of potential are assigned. Backward differencing of the time derivatives is used with the initial time step, and central differencing is used subsequently.

The semiconfining layers, which are represented by the finite elements, are simultaneously solved for changes in pressure by a fully three-dimensional treatment of the nodal equations. EQSOLV is the matrix inversion algorithm used in FE3DGW to solve the large, sparse, nonbanded system of equations. In this algorithm, row pivoting is about the minimum nonzero element; whereas, the pivot column is about the largest absolute element in the pivot row.

The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
- The porosity and hydraulic conductivity are constant with time.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- The storage term is a function of the compressibility of the fluid and porous medium only.
- The medium is fully saturated.

- Hydraulic conductivity principal axes are aligned parallel to the coordinate axes.

CODE INPUT: Input requirements include specification of geologic stratigraphy, liquid and media properties, positioning and rates of manmade aquifer stresses, boundary conditions at the areal extent of the aquifer, and initial conditions for dynamic simulations. Specifically, these requirements include:

- Geologic stratigraphy
  - Number of distinct geologic layers
  - Total aquifer thickness
  - Elevation of geologic media interfaces
  - x,y coordinates of elevation data

- Liquid properties
  - Viscosity
  - Density
  - Temperature profile

- Media properties
  - Intrinsic permeability or hydraulic conductivity
  - Porosity
  - Storativity

- Manmade stresses
  - x,y coordinates of wells
  - Screened elevation
  - Rate of withdrawal or injection

- Boundary conditions
  - Water levels of hydrologically significant water bodies (e.g., streams, lakes, oceans)
  - Nodal fluxes due to pumping
  - Vertical infiltration
  - Lateral recharge defined by data or modeling conducted on a larger scale
  - Lateral no-flow boundaries defined by groundwater divides or impermeable media

- Initial conditions for dynamic simulations
  - Water table elevations in unconfined zones
  - Spatial distribution of pressure in confined zones.

Two- and three-dimensional plotting routines are included in the FE3DGW technology for the purpose of visualizing any obvious errors in the input data. Inconsistency in the entered data is also monitored by built-in consistency checks and diagnostics.

CODE OUTPUT: Results are in the form of:

- Flow field;

- Flow paths; and

- Travel times.

Various levels of output detail are available:

- Geometric description;
- Number of nodes;
- Types of nodes;
- Dimensions;
- Surface node coordinates;
- Input data echo; and
- Output of all nodes and elements at selected time levels.

Written output can be directed to the line printer or disk. Plotted output is in the form of contour maps, grid displays, and three-dimensional, dependent-variable surfaces.

COMPILATION REQUIREMENTS: FE3DGW is written in FORTRAN IV and is currently being run on a VAX 11/780. The code is generally compatible with most all mainframe or virtual memory machines.

Current program limits are:

- 768 surface nodes;
- 2560 system nodes;
- 20 layers per well log;
- 99 materials;
- 768 potential boundary conditions;
- 128 stream nodes;
- 20 nonzero element nodes;
- 2048 unknown nodes;
- 128 nonzero element bandwidth;
- 768 surface elements;
- 2000 system elements; and
- 70 time steps

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Verification analysis of the three-dimensional model was accomplished using two-dimensional or quasi-three-dimensional analytical solutions. These include radial confined and leaky aquifer solutions given by Theis (ref. 2) and Hantush (ref. 4), respectively, and also the two-dimensional analytic solution PATHS (ref. 5).

FE3DGW has been applied extensively to the groundwater system beneath Long Island, New York (ref. 6). The Long Island groundwater basin is one of the most intensively monitored systems in the U.S.

The model has also been applied to the groundwater system at Sutter Basin, California, where it has been inferred (ref. 7) that fresh water which is recharging at Sutter Buttes rises through the Sutter Basin fault, creating a salt-water mound.

The model has been used on several other occasions to better understand the groundwater flow portion of a contaminant transport application (ref. 8, 9, and 10).

DOCUMENTATION/REFERENCES:

Gupta, S.K.; Cole, C.R.; Bond, F.W. (1979) Finite element three dimensional ground water (FE3DGW) flow model formulation, program listings and user's manual. Pacific Northwest Laboratory Report PNL-2939.

Theis, C.V. (1935) The relation between the lowering of the piezometric surface and the rate and duration of discharge of a well using groundwater storage. Trans. Amer. Geophys. Union 2:519-524.

Jacob, C.E. (1950) In: Rouse, H., ed. Engineering Hydraulics. New York, NY: John Wiley and Sons, pp. 321-386.

Hantush, M.S. (1960) Modification of theory of leaky aquifers. J. Geophys. Res. 65:3713-3725.

Nelson, R.W.; Schur, J.A. (1980) PATHS groundwater hydrogeological model. Pacific Northwest Laboratory Report PNL-3162.

Gupta, S.K.; Pinder, G.F. (1978) Three-dimensional finite element model for multilayered ground-water reservoir of Long-Island, New York. Department of Civil Engineering, Princeton University, Princeton, NJ.

Gupta, S.K.; Tanji, K.K. (1976) A three-dimensional Galerkin finite element solution of flow through multiaquifers in Sutter Basin, California. Water Resour. Res. 12(2):155-162.

Bond, F.W.; Eddy, C.M. (1985) Remedial action modeling assessment, Western Processing Site, Kent, Washington. Prepared for the U.S. Environmental Protection Agency, Region X, Seattle, WA.

Schalla, R.; McKown, G.L.; Meuser, J.M.; Parkhurst, R.G.; Smith, C.M.; Bond, F.W.; English, C.J. (1984) Source identification contaminant transport simulation and remedial action analysis, Anniston Army Depot, Anniston, Alabama. Prepared for Commander, Anniston Army Depot, Anniston, AL.

Cole, C.R.; Bond, F.W.; Brown, S.M.; Dawson, G.W. (1983) Demonstration/ application of groundwater modeling technology for evaluation of remedial action alternatives. Prepared for the U.S. Environmental Protection Agency, Municipal Environmental Research Laboratory, Cincinnati, OH.

SOURCE: FE3DGW was written by S. K. Gupta, C. R. Cole, and F. W. Bond as a result of research conducted by Pacific Northwest Laboratory and supported by the Waste Isolation Safety Assessment Program (WISAP). FE3DGW is a derivative of DAVIS/FE which was also written by S. K. Gupta.

CODE NAME: FLUMP

PHYSICAL PROCESSES: Predicts two-dimensional groundwater flow.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite element, and a mixed explicit-implicit point iterative solution.

DESCRIPTION: The FLUMP model evolved from the TRUST model, although it has been modified considerably by S. P. Neuman. It is considerably easier to use on groundwater flow problems than is TRUST, although it is restricted to two-dimensional flow in either vertical or horizontal planes. FLUMP uses a finite-element numerical scheme which has been shown to represent only a small change from the original approach used in TRUST.

CODE INPUT: Standard saturated zone hydrologic parameters.

CODE OUTPUT: Head distribution at each time step.

COMPILATION REQUIREMENTS: FLUMP is written in FORTRAN and is operational on a CDC system.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Fogg, G.E.; Simpson, E.S.; Neuman, S.P. (1979) Aquifer modeling by numerical methods applied to an Arizona groundwater basin. PB 298962, National Technical Information Service, Springfield, VA, 140 pp.

Narasimhan. T.N.; Neuman, S.P.; Edwards, A.L. (1977) Mixed explicit-implicit iterative finite element scheme for diffusion-type problems. 2. Solution strategy and examples. Int. J. Numer. Methods Eng. II:235-244.

Neuman, S.P.; Narasimhan, T.N. (1977) Mixed explicit-implicit iterative finite element scheme for diffusion-type problems. 1. Theory. Int. J. Numer. Methods Eng. II:309-323.

Neuman, S.P.; Narasimhan, T.N.; Witherspoon, P.A. (1977) Application of mixed explicit finite element method to nonlinear diffusion type problems. In: Pinder, G.F.; Gray, W.E., eds. Proceedings of the First International Conference on Finite Elements in Water Resources, Princeton, NJ, Pentech, pp. 1.153-1.185.

SOURCE: This code was developed by S. P. Neuman of the University of Arizona, Department of Hydrology. The code is in the public domain.

CODE NAME: FRESURF 1 & 2

PHYSICAL PROCESSES: Predicts two-dimensional and axisymmetric flow.

DIMENSIONALITY: Two dimensional and axisymmetric.

SOLUTION TECHNIQUE: Finite element.

DESCRIPTION: In this two-dimensional model, the specifics of the free-surface boundary as described by Neuman are incorporated into the finite-element solution scheme used. 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 or the potential, with respect to time, is combined with specific free-boundary conditions that 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 nonsteady flow with the free surface. The regular finite-element approach, based on 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 used.

CODE INPUT: Standard saturated zone hydrologic parameters.

CODE OUTPUT: Head distribution at each time step.

COMPILATION REQUIREMENTS: FRESURF 1 and 2 are written in FORTRAN and operational on a CDC system.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Neuman, S.P.; Witherspoon, P.A. (1971) Analysis of nonsteady flow with a free surface using the finite element method. Water Resources Research, 7(3):611-623.

SOURCE: FRESURF 1 and 2 were written by S. P. Neuman of the University of Arizona, Department of Hydrology. The code.is in the public domain.

CODE NAME: TERZAGI

PHYSICAL PROCESSES: TERZAGI solves for three-dimensional fluid flow with one-dimensional consolidation in saturated systems.

DIMENSIONALITY: Three dimensional.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: This model numerically simulates the movement of water in saturated deformable porous media. The theoretical model considers a general three-dimensional field of flow in conjunction with a one-dimensional vertical deformation field. The governing partial differential equation expresses the conservation of fluid mass in an elemental volume that has a constant volume of solids. The numerical solution is based on the integrated finite difference method (IFDM), which is very convenient for handling multi-dimensional heterogeneous systems composed of isotropic materials.

The present computer program is based on modifications of earlier versions of TRUST and TRUMP.

CODE INPUT: Standard saturated zone hydrologic parameter plus consolidation parameters.

CODE OUTPUT: Head distribution, consolidation information.

COMPILATION REQUIREMENTS: TERZAGI was written in FORTRAN IV and implemented on a CDC system.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Narasimhan, T.N.; Witherspoon, P.A. (1976) An integrated finite difference method for analyzing fluid flow in porous media. Water Resources Research 12(1).

SOURCE: The code was developed by T. N. Narasimhan of the University of California. This code is in the public domain.

CODE NAME: USGS2D

PHYSICAL PROCESSES: Saturated groundwater flow in a confined, unconfined, or combined confined and unconfined aquifer.

DIMENSIONALITY: Two dimensional (x-y or x-z cartesian).

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: USGS2D is a finite-difference saturated flow code. It is restricted to two-dimensional (areal) flow, but has many options. USGS2D provides the user with a variety of options for 1) groundwater flow conditions; 2) source terms; 3) numerical solution techniques; and 4) input-output. The options for groundwater flow conditions include:

- confined conditions;
- unconfined conditions; and
- combined confined and unconfined conditions.

Variations of source terms include:

- transient leakage from confining beds;
- steady leakage from confining beds;
- recharge;
- pumping wells; and
- evapotranspiration.

The program is fairly general. The flow field is represented as a two-dimensional grid. The size of the grid blocks is variable to allow the desired level of spatial detail. Variable time steps are also allowed.

The major variable is hydraulic head, although drawdowns may be computed from the initial head condition.

The model was designed primarily for areal simulations but can be used for some cross-sectional problems. Generally this is done using the artesian option. An example of a cross-sectional simulation is provided in the documentation.

A minor problem is that the code is programmed such that two extra columns and two extra rows are required to border the gridded area. This results in some additional work when preparing input data. It is also difficult to convert the code to run on non-IBM machines.

USGS2D is designed for most types of geological media where two-dimensional flow in a porous medium can be assumed. The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.

- Vertically averaged properties may be used.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- Transmissivity principal components are aligned along coordinate axes.
- Linear evapotranspiration.
- Maximum evapotranspiration rate may not vary spatially.
- The porosity and hydraulic conductivity are constant with time.

CODE INPUT: USGS2D may read single or multiple data sets. The contents of a data set are described in Table A-1.

CODE OUTPUT: USGS2D prints the following: 1) all input; 2) time-step information; 3) mass-balance information; 4) matrix-iteration information; and 5) computed hydraulic head or drawdown.

COMPILATION REQUIREMENTS: USGS2D was programmed in FORTRAN IV for use on an IBM machine. It has been successfully adapted for use on CDC and UNIVAC machines as well. Model results can be presented on the line printer (rows should be numbered in the short dimension) and pen plotters with a program that utilizes the graphical display software available from the U.S. Geological Survey Computer Center Division. In addition, included in the model are options for reading input data from a disk and writing intermediate results on a disk.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: USGS2D has been compared to analytical solutions including those for leaky aquifers. It has also been used to simulate several hypothetical problems where detailed mass balance calculations were made.

This code has been the work horse of the U.S. Geological Survey for more than ten years. It has been applied to numerous sites throughout North America. Most of these applications have dealt with water supply problems associated with relatively shallow aquifers. Some of the field problems include the Washington, D.C., area (ref. 3), west-central Minnesota (ref. 4), and Nova Scotia (ref. 5).

DOCUMENTATION/REFERENCES:

Documentation (refs. 1 and 2) for USGS2D is available in two government publications.

Trescott, P.C.; Pinder, G.F.; Larson, S.P. (1976) Finite-difference model for aquifer simulation in two dimensions with results of numerical experiments. U.S. Geological Survey, Techniques of Water-Resources Investigations, Book 7, Chapter C1.

Table A-1. Summary of Major Data Requirements for Various Flow-Condition Options and Source Terms in USGS2D

Flow Conditions	Source Conditions			
	Aquifer Parameters	Leakage	Recharge	Evapotranspiration
Confined	Transmissivity Storage coefficient	Hydraulic conductivity of confining bed Head in source aquifer Confining bed thickness Confining bed specific storage (= 0 for steady leakage)	Recharge rate	
Unconfined	Hydraulic conductivity Aquifer bottom Specific Yield	Same as above; adjustments made internally	Recharge rate	Land elevation Max E-T rate E-T cut-off depth
Combined Confined and Unconfined	Hydraulic conductivity Aquifer bottom Aquifer top Storage coefficients Specific yield	Same as above; adjustments made internally	Recharge rate	Land elevation Max E-T rate E-T cut-off depth

Larson, S.P. (1979) Direct solution for the two-dimensional ground-water flow model. U.S. Geological Survey, Open-File Report 78-202.

Papadopulos, S.S.; Bennett, R.R.; Mack, F.K.; Trescott, P.C. (1984) Water from the coastal plain aquifers in the Washington, D.C., metropolitan area. U.S. Geological Survey Circular 697.

Larson, S.P.; McBride, M.S.; Wolf, R.J. (1975) Digital models of a glacial outwash aquifer in the Pearl-Sallie Lakes Area. U.S. Geological Survey Water-Resources Investigations 40-75.

Pinder, G.F.; Bredehoeft, J.D. (1968) Application of the digital computer for aquifer evaluation. Water Resour. Res. 4:(5):1069-1093.

SOURCE: USGS2D was developed at the U.S. Geological Survey and is described in Techniques of Water-Resources Investigations, Book 7, Chapter C1, by P. C. Trescott, G. F. Pinder, and S. P. Larson. The code is in the public domain. In addition, the USGS offers some support for certain users and applications.

CODE NAME: USGS3D -- Modular

PHYSICAL PROCESSES: Predicts groundwater flow in confined/unconfined aquifers.

DIMENSIONALITY: Three-dimensional.

SOLUTION TECHNIQUE: Numerical, finite-difference.

DESCRIPTION: Groundwater flow within the aquifer is simulated using a block-centered finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of confined and unconfined. Flow from external stresses, such as flow to wells, areal recharge, evapotranspiration, flow to drains, and flow through riverbeds, can also be simulated. The finite-difference equations can be solved using either the Strongly Implicit Procedure or Slice-Successive Overrelaxation.

The modular structure consists of a main program and a series of highly independent subroutines called "modules." The modules are grouped into "packages," each package addresses a specific feature of the hydrologic system.

CODE INPUT: Standard saturated zone hydrologic parameters.

CODE OUTPUT: Head distribution at each time step.

COMPILATION REQUIREMENTS: The program is written in FORTRAN '66 and will run without modification on most computers which have a FORTRAN '66 compiler. It will also run, without modification, with most extended FORTRAN '77 compilers and with minor modifications on standard FORTRAN '77 compilers.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

McDonald, M.G.; Harbaugh, A.W. (1984) A modular three-dimensional finite-difference groundwater flow model. U.S. Geological Survey Open-File Report 83-875.

SOURCE: The code was written by Michael McDonald and Arlen Harbaugh of the U.S. Geological Survey. This code is in the public domain.

CODE NAME: USGS3D -- Trescott

PHYSICAL PROCESSES: Fully three-dimensional or quasi-three-dimensional saturated groundwater flow in confined, unconfined, or combined confined and unconfined aquifers.

DIMENSIONALITY: Fully three-dimensional, quasi-three-dimensional.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: USGS3D simulates three-dimensional flow in a porous medium which may be heterogeneous and anisotropic and have irregular boundaries. The uppermost hydrologic unit may have a free surface. The stresses considered are wells and recharge from precipitation.

One or more layers of nodes can be used to simulate each hydrogeologic unit. It it is reasonable to assume that storage is negligible in a confining bed and that horizontal components of flow can be neglected, the effects of vertical leakage through a confining bed can be incorporated into the vertical component of the anisotropic hydraulic conductivity of adjacent aquifers.

A major advantage of this code is that it can be used in a fully three-dimensional mode or it can be reduced to a quasi-three-dimensional model in terms of the equations being solved and computer memory requirements. This is accomplished by using a sequence of two-dimensional (areal) groundwater flow models to represent aquifers. These models are coupled by terms representing flow through intervening confining beds to form a quasi-three-dimensional model. This latter model converges to a solution much faster than the fully three-dimensional model because all equations are solved simultaneously. It should be noted, however, that the leakage in this quasi-three-dimensional model is steady, that is, it ignores storage. For long-term simulations which approach steady state, this type of leakage is adequate.

The flow field can be represented as a three-dimensional grid or a sequence of two-dimensional grids. The program is fairly general in that the size of the grid blocks is variable to allow the desired level of spatial detail. Variable time steps are also allowed.

The major variable is hydraulic head, although drawdowns may be computed from the initial head condition. The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
- The porosity and hydraulic conductivity are constant with time.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- Hydraulic conductivity principal components are aligned with Cartesian coordinate system.
- Steady leakage from confining beds can be incorporated into anisotropic hydraulic conductivity of adjacent aquifers.

CODE INPUT: The data required to run USGS3D includes finite-difference data, such as spacing and physical data. The physical data includes:

- initial heads;
- boundary conditions;
- storage coefficient distribution;
- transmissivity distribution; and
- recharge rate.

If the upper unit is unconfined, then hydraulic conductivity and the elevation of the bottom of the water table layer is read in place of transmissivity.

CODE OUTPUT: USGS3D prints the following: 1) all input; 2) time-step information; 3) mass-balance information; 4) matrix-iteration information; and 5) computed hydraulic head or drawdown.

COMPILATION REQUIREMENTS: USGS3D was programmed in FORTRAN IV for use on an IBM machine, using some machine-dependent features.

Rows should be numbered in the short dimension for plotting maps on the line printer or for plotting data with an X-Y drum plotter. The core requirements and computation time are proportional to the number of nodes representing the porous medium.

To reduce the number of cards that must be read with each run, the program includes options to place the arrays on disk and, on subsequent runs, read the data from disk rather than from cards.

The documented program was designed to take advantage of certain features of an IBM machine. Because of this, there are difficulties in converting the code to a non-IBM machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The code has been applied to several field problems and code results have been compared with analytical solutions. USGS3D does have a detailed mass balance to ensure that the solution has converged.

This code has been applied to several field problems, including flow problems associated with mining, hazardous waste, and radioactive waste (Columbia Plateau). As an example of a field application of this code to a mining problem, see ref. 3.

DOCUMENTATION/REFERENCES:

Trescott, P.C. (1975) Documentation of finite-difference model for simulation of three-dimensional ground-water flow. U.S. Geological Survey Open-File Report 75-438.

Trescott, P.C.; Larson, S.P. (1976) Documentation of finite-difference model for simulation of three-dimensional ground-water flow. U.S. Geological Survey Open-File Report 76-591, supplement to Open-File Report 75-438.

Weeks, J.B.; Leavesley, G.H.; Wleder, F.A.; Saulneir, G.J., Jr. (1984) Simulated effects of oil-shale development on the hydrology of Piceance Basin, Colorado. U.S. Geological Survey Professional Paper 908.

SOURCE: USGS3D was developed at the U.S. Geological Survey and is described in a series of reports by P. C. Trescott and S. P. Larson. The code is in the public domain. In addition, the USGS offers some support for certain users and applications.

CODE NAME: VTT

PHYSICAL PROCESSES: Predicts the transient or steady-state hydraulic head distribution and provides water flow paths and travel times.

DIMENSIONALITY: Two dimensional (x-y cartesian).

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: The model is capable of calculating water flow in a multilayered aquifer system. The system may be confined, unconfined, or semiconfined. The main simplifying assumption transforms a three-dimensional system to a layered two-dimensional system with interaquifer transfer via a potential-driven leakage term. The mathematical model which utilizes this set of simplifying assumptions is the multi-aquifer formulation of the Boussinesq equations. VTT uses a horizontal, two-dimensional, finite-difference approach for saturated flow in each aquifer. The code may analyze flow in such a system for a variety of initial and boundary conditions for steady or non-steady flow.

The velocity field in the porous medium is part of the output of VTT. The analysis of the flow field is the first stage in predicting the transport of contaminants in a porous medium. The output of the flow field could subsequently be used to develop inputs for such transport codes as MMT or FEMWASTE.

For numerical formulations, a horizontal x-y coordinate grid system is adopted with uniform nodal spacing. Standard finite-difference approximations and a fully implicit representation of the time derivative are used.

When considering confined flow, the compressibility effects of the fluid and matrix are incorporated, but they are neglected when considering unconfined flow. This assumption is quite valid as long as the specific yield is not of the same magnitude as the specific storage.

The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
- The porosity and hydraulic conductivity are constant with time.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- Hydraulic conductivity and effective porosity can be represented by the vertically averaged values and are isotropic throughout the region but may be inhomogeneous.
- The free-surface slope and the aquifer bottom slope are both slight (<5o).
- Vertical velocities are small and can be neglected.
- Flow in the capillary finge is neglected.
- Seepage surfaces cannot be handled and are neglected.

CODE INPUT: Inputs to VTT include:

- total stress or recharge at each node;
- aquifer top elevation;
- aquifer bottom elevation;
- initial aquifer potential;
- aquifer storage coefficient;
- interaquifer transfer (leakage) coefficient; and
- aquifer hydraulic conductivity (or transmissivity) at each node.

CODE OUTPUT: The output for VTT is the new spatial variation of potential throughout the aquifers. From this potential distribution in conjunction with other input data, the following information can be calculated:

- groundwater velocities;
- groundwater flow paths;
- travel times; and
- new recharge/discharge relationships along streams and rivers.

Types of model output that can be produced include:

- Contour maps of:
  - equal potential
  - equal drawdown
  - equal transmissivity
- Three-dimensional projection plots of:
  - potential
  - drawdown
  - transmissivity
- Cross-sectional plots showing aquifer top, aquifer bottom, and aquifer potential.
- Flow path plots with associated listings of travel times.
- Numerical listings of the input data or calculated potentials.
- Difference maps showing the node-by-node predictions of potential changes.

COMPILATION REQUIREMENTS: VTT is written in FORTRAN IV-PLUS. The code can be run on a PDP 11/70 or VAX machines. The code was converted to a CDC machine by Intera, Inc.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: VTT has been compared with solutions from a more general three-dimensional model, FE3DGW, and a model which uses an analytical solution, PATHS.

DOCUMENTATION/REFERENCES:

Reisenauer, A.E. (1979) Variable thickness transient groundwater flow model (VTT), formulation, user's manual and program listings. Pacific Northwest Laboratory Report PNL-3160-1, PNL-3160-2, and PNL-3160-3.

Gupta, S.K.; Cole, C.R.; Bond, F.W. (1979) Finite element three dimensional groundwater (FE3DGW) flow model, formulation, program listings and user's manual. Pacific Northwest Laboratory Report PNL-2939.

Kellogg, O.C. (1954) Foundations of potential theory. Dover, NY.

SOURCE: VTT was developed at Battelle, Pacific Northwest Laboratory. The work was supported by the Department of Energy. The code is in the public domain.

CODE NAME: V3

PHYSICAL PROCESSES: Predicts groundwater flow in heterogeneous anisotropic aquifers under a variety of flow conditions.

DIMENSIONALITY: Two-dimensional (x-y cartesian).

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: This series of computer programs simulates one- or two-dimensional nonsteady-state flow problems in heterogeneous anisotropic aquifers under water table, nonleaky, and leaky artesian conditions. Multiple-aquifer problems with leakage between aquifers can also be treated. These programs cover time-varying pumpage from wells, natural or artificial recharge rates, the relationships of water exchange between surface waters and the groundwater reservoir, the process of groundwater evapotranspiration, the mechanism of possible conversion of storage coefficients from artesian to water table conditions, and the multiple-aquifer problem.

The program is fairly general. One- or two-dimensional grids, or sequences of two-dimensional grids, may be used. The size of the grid blocks are variable to allow the desired level of spatial detail. Variable time steps are also allowed. The code considers several different flow conditions such as hydraulic conductivity, storage properties, leakage properties, and recharge properties.

V3 is programmed in modular fashion that allows relatively convenient modification. In general, the modules contain logical work tasks. The modules, however, are not contained in subroutines; everything is contained in the main program.

The main assumptions of the code are:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
- The porosity and hydraulic conductivity are constant with time.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- Vertically averaged properties can be used.
- Transmissivity principal components are aligned with cartesian coordinate system.
- Leakage is steady state.
- Linear evapotranspiration.

CODE INPUT: Input for the basic aquifer simulation program includes:

- parameter and default value cards;
- array data;

- transmissivity;
- storage coefficient;
- initial hydraulic heads; and
- pumpages.

With modifications to the program, additional data are read as follows:

Option	Additional Data
Variable Pumping Rates	Time and pumping rate of each period
Leaky Artesian Conditions	Vertical hydraulic conductivity and thickness of confining bed; head difference across confining bed
Induced Infiltration	Same as leaky artesian conditions plus areas of the stream bed
Evapotranspiration	Land surface elevation; elevations of the water table below which ET ceases; maximum ET rate
Storage Coefficient Conversion	Elevation of aquifer top; water table storage coefficient
Water Table Conditions	Water table storage coefficient; elevation of aquifer bottom

CODE OUTPUT: The primary outputs of V3 are hydraulic head or drawdowns. There are options for displaying these in a readable fashion, such as time-water level graphs.

COMPILATION REQUIREMENTS: The computer programs were written in FORTRAN IV for use on an IBM 360 system model 75 with a G-level compiler. However, the programs will operate, with modifications, on other computers. Also, these computer programs are written so that they will operate with any consistent set of units.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: V3 is one of the most widely used groundwater flow codes. It has been compared to several analytical solutions, including those by Theis, Hantush, and Jacob.

DOCUMENTATION/REFERENCES:

Prickett, T.A.; Lonnquist, C.G. (1971) Selected Digital Computer Techniques for groundwater resource evaluation. Illinois State Water Survey, Bulletin 55.

McDonald, M.G.; Fleck, W.B. (1978) Model analysis of the impact on groundwater conditions of the Muskegon County waste-water disposal system, Michigan. U.S. Geological Survey Open-File Report 78-99.

SOURCE: V3 was developed at Illinois State Water Survey. The code is in the public domain.

NUMERICAL SOLUTE TRANSPORT
(SATURATED/UNSATURATED)

CODE NAME: FEMWASTE1 (Finite-Element Model of Waste Transport)

PHYSICAL PROCESSES: Predicts waste transport through saturated-unsaturated porous media under dynamic groundwater conditions.

DIMENSIONALITY: Two-dimensional (x-y, x-z cartesian).

SOLUTION TECHNIQUE: Numerical, finite-element.

DESCRIPTION: FEMWASTE1 is an upgraded version of the FEMWASTE code developed by Yeh and Ward for subsurface transport. It is a transport-only code that requires fully specified hydrodynamics as part of the input data set. FEMWATER1, a flow model using an identical numerical representation of the problem domain, creates a geometric and hydrodynamic data file expressly for FEMWASTE1.

FEMWASTE1 is capable of transient, two-dimensional simulations of pollutant transport in saturated and unsaturated porous media. The model includes the following transport processes:

- advection;
- hydrodynamic dispersion;
- sorption;
- first-order decay; and;
- source/sink.

FEMWASTE1 uses quadrilateral bilinear elements for spatial discretization of the porous media. Solution is by the finite element weighted residual method. Two finite element weighting techniques are available: Galerkin and upwind.

The option of "lumping" the finite element mass matrix into a type of finite difference unit mass matrix by scaling is also available. In some situations the lumping technique has been more accurate. Included in the FEMWASTE1 formulation is the option of three time-stepping techniques:

1) central difference;

2) backward difference; and

3) mid-difference.

Regardless of the technique selected, Gaussian elimination is used to invert the resulting matrices.

With the options of weighting, lumping, and time stepping, 12 different computational approaches are possible with FEMWASTE1.

FEMWASTE1 is designed to be applied uncoupled from the flow field calculations. This design implicitly assumes that transport processes do not affect the fluid transport. The model is applied to a single chemical species without considering the effects of other chemicals that may be present in the

porous media. The only irreversible reaction in FEMWASTE1 is in the first-order decay process where degradation is assumed to be directly proportional to the total pollutant concentration (including dissolved and adsorbed phases). FEMWASTE1 does not explicitly account for biological uptake or other degradation mechanisms, although these effects can be included approximately by adjusting the decay constant. Transformation and loss mechanisms can be represented by the source/sink term local to each element. Chemical sorption is assumed to be a reversible fast-exchange reaction that attains local equilibrium within a single time interval according to a linear isotherm. The distribution coefficient, Kd, is moisture independent in FEMWASTE1. This assumption restricts the model application to cases where all soil grains are effective in the adsorption process. The calculated retardation factor, however, is an inversely dependent function of the moisture content.

CODE INPUT: FEMWASTE1 requires standard material and aquifer properties:

- adsorption distribution coefficient;
- bulk density;
- longitudinal dispersivity;
- transverse dispersivity;
- decay constant;
- porosity; and
- modified coefficient of compressibility.

Aquifer characteristics can be entered on a regional basis or can be specific to a given element.

Three types of boundary conditions are possible with FEMWASTE1:

1) Dirichlet, specifications of time-varying concentrations at a particular element;

2) Neuman, specification of time-varying waste fluxes at a particular element; and

3) Cauchy, waste-flux boundary conditions that are specific to inflow boundaries.

Initial conditions are concentrations of pollutant in the porous media.

An error checker is present in FEMWASTE1 to ensure that the input data are correct. When errors are detected, execution is stopped.

CODE OUTPUT: Output from FEMWASTE1 consists of formatted line-printer listings of concentrations at specified locations and times. An auxiliary storage device file is created for post processing on local hardware.

COMPILATION REQUIREMENTS: FEMWASTE1 is written in FORTRAN. Current limits on the program are:

- 595 nodes;
- 528 elements;
- 500 time steps;
- 29 water boundary conditions;
- 199 boundary elements;
- 200 boundary nodes;
- 99 rainfall seepage element sides; and
- 100 rainfall seepage element sides.

FEMWASTE1 is designed to be applied in a batch mode. The model is constructed in a modular fashion with one main program and 15 subroutines. Efficient storage of the banded matrix arrays are used in FEMWASTE1. Annotation of the source listing is good with short descriptions and identified computations. Conversion to the VAX 11/780 is straightforward.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: A sample problem of transport from a seepage pond reported by Duguid and Reeves was used to compare the simulation by the original computer codes with that by the new waste-transport code coupled with the revised water-flow code. The code is in the public domain.

DOCUMENTATION/REFERENCES:

Bear, J. (1972) Dynamics of fluids in porous media. New York, NY: American Elsevier.

Duguid, J.O.; Reeves, M. (1976) Material transport in porous media: a finite element Galerkin model. ORNL-4928, Oak Ridge National Laboratory, Oak Ridge, TN.

Reeves, M.; Duguid, J.O. (1975) Water movement through saturated- unsaturated porous media: a finite-element Galerkin model. ORNL-4927, Oak Ridge National Laboratory, Oak Ridge, TN.

Yeh, G.T. (1982) Training course no. 2: the implementation of FEMWASTE (ORNL-5601) computer program. ORNL/TM-8328, NUREG/CR-2706, U.S. Nuclear Regulatory Commission, Washington, DC.

Yeh, G.T.; Ward, D.S. (1981) FEMWASTE: a finite-element model of waste transport through saturated-unsaturated porous media. ORNL-5601, Oak Ridge, National Laboratory, Oak Ridge, TN.

Yeh, G.T.; Ward, D.S. (1980) FEMWATER: a finite-element model of water flow through saturated-unsaturated porous media. ORNL-5567, Oak Ridge National Laboratory, Oak Ridge, TN.

SOURCE: FEMWASTE was developed at Oak Ridge National Laboratory and is described in Report No. ORNL-5601 by G. T. Yeh and D. S. Ward. It is an extension of work done by Duguid and Reeves.

CODE NAME: PERCOL

PHYSICAL PROCESSES: Predicts the movement of a solute through a soil column.

DIMENSIONALITY: Unknown.

SOLUTION TECHNIQUE: Numerical, Newton-Raphson method.

DESCRIPTION: PERCOL has been developed to simulate the movement of radionuclides through porous media as a function of measurable chemical parameters of the media. System parameters include soil type, radionuclide type, waste composition, flow rate, column length, and soil saturation.

CODE INPUT: Standard transport parameters.

CODE OUTPUT: Predictions of concentrations.

COMPILATION REQUIREMENTS: PERCOL is written in FORTRAN and implemented on an IBM 360 machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: Laboratory column studies have been conducted to verify the model.

DOCUMENTATION/REFERENCES:

Owen, P.T. An inventory of environmental impact models relating to energy technologies. ORNL/EIS-147, Oak Ridge National Laboratory, Oak Ridge, TN.

Routson, R.C.; Serne, R.J. (1972) One-dimensional model of the movement of tracer radioactive solute through soil columns: the PERCOL model. BNWL-1718, Battelle, Pacific Northwest Laboratories, Richland, WA.

SOURCE: PERCOL was written by R. C. Routson of Argonne National Laboratory and R. J. Serne of Battelle, Pacific Northwest Laboratories. The code is in the public domain.

CODE NAME: SATURN

PHYSICAL PROCESSES: Predicts saturated-unsaturated flow and radioactive radionuclide transport.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: SATURN is a two-dimensional finite-element model developed to simulate fluid flow and solute transport processes in variably saturated porous media. The model solves the flow and transport equations separately. Transport mechanisms considered include advection, hydrodynamic dispersion, adsorption, and first-order decay.

The flow equation is discretized using the Galerkin finite-element method. Nonlinearity is treated using either Picard or Newton-Raphson iterations. The transport equation is discretized using an upstream-weighted finite-element method designed to alleviate the problem of numerical oscillations. Simple rectangular and triangular elements are used. The combination of such elements enables flow regions of complex geometry to be modeled accurately. A highly efficient "influence coefficient" technique is used to generate element matrices. This technique avoids numerical integration and leads to a reduction in CPU time required for element matrix generation. For rectangular elements, the saving of CPU time

- prescribed values of nodal fluid flux;
- longitudinal dispersivity;
- transverse dispersivity;
- molecular diffusion coefficients;
- decay coefficient;
- retardation coefficient;
- initial inventory of solute;
- leach duration;
- prescribed values of concentration; and
- prescribed values of solute flux.

CODE OUTPUT: The primary line printer output from the flow model of SATURN includes nodal values (at various time levels) of pressure head and element centroidal values of Darcy velocity components and saturation at various time levels. SATURN allows the user to select the fluid mass balance calculation option. This budget contains information about the net flow rate of fluid due to boundary fluxes, sources, and sinks; the rate of fluid accumulation in the entire flow domain; the mass balance error; and the cumulative fluid storage up to the current time.

The primary line printer output of the transport model of SATURN includes nodal values (at various time levels) of solute concentration. SATURN also allows the user to select the solute mass balance calculation option. If the solute mass balance budget is activated, information about the total dispersive and advective fluxes; the net rate of material accumulation taking into account storage, adsorption, and decay; the mass balance error; the cumulative mass of solute still remaining in the porous medium at the current time; and the cumulative mass decay up to the current time value will be printed at the end of each time step.

COMPILATION REQUIREMENTS: SATURN is written in FORTRAN with versions existing on the following computer systems:

- PRIME;
- DEC VAX 11/780; and
- CDC 7600.

The code is written in double precision (eight-byte decimal words). The code treats the transport processes as an uncoupled phenomenon from the flow processes; thus, two successive applications of SATURN are necessary to simulate flow and transport.

Current problem limits:

- 500 nodal points;
- 450 elements;
- 20 materials;
- 99 Dirichlet boundary conditions;
- 99 flux boundary conditions;
- 40 semi-bandwidth for global matrix;
- 10 time-dependent Dirichlet boundary nodes;
- 10 time-dependent flux boundary nodes;
- 20 entry pairs for relative permeability versus saturation; and
- 20 entry pairs for pressure head versus saturation.

Due to the manner in which these limits are prescribed in the code, changes in dimension can require the modification of common blocks, in almost every subroutine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: The code has been verified against several test problems and against UNSAT2.

DOCUMENTATION/REFERENCES:

Huyakorn, P.S.; Thomas, S.D.; Mercer, J.W.; Lester, B.H. (1983) SATURN: a finite element model for simulating saturated-unsaturated flow and radioactive radionuclide transport. Prepared by Geotrans for the Electric Power Research Institute, Palo Alto, CA.

SOURCE: SATURN is a proprietary code. It was developed by P. S. Huyakorn, S. D. Thomas, J. W. Mercer, and B. H. Lester, all of Geotrans, Incorporated.

CODE NAME: SEGOL

PHYSICAL PROCESSES: Predicts contaminant transport and flow for combined saturated and partially-saturated flow systems.

DIMENSIONALITY: Three dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The transport equations are solved using a Galerkin finite-element approach. 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 uses 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 indicated that a spatial discretization of a few centimeters may be necessary for some problems.

CODE INPUT: Standard transport parameters.

CODE OUTPUT: Predictions of head and concentration.

COMPILATION REQUIREMENTS: SEGOL is written in FORTRAN.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: SEGOL has been verified by comparison to field data.

DOCUMENTATION/REFERENCES:

Segol, G.A. (1976) Three-dimensional Galerkin finite element model for the analysis of contaminant transport in variably saturated porous media -- user's guide. Department of Earth Sciences, University of Waterloo, Waterloo, Ontario, Canada, June.

Segol, G.A. (1977) A three-dimensional Galerkin-finite element model for the analysis of contaminant transport in saturated-unsaturated porous media. In: Gray, W.G.; Pinder, G.F., eds., Finite elements in water resources, (Proceedings of the First International Conference, July, 1976).

SOURCE: SEGOL was developed by G. A. Segol of Bechtel Corporation. The code is in the public domain.

CODE NAME: SUMATRA-I

PHYSICAL PROCESSES: Predicts the simultaneous flow of water and solutes transport in a vertical soil profile under transient saturated-unsaturated conditions.

DIMENSIONALITY: One dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: SUMATRA-I is based on a Hermitian (cubic) finite-element solution of the governing transport equations. The model includes such processes as linear equilibrium adsorption and zero- and first-order decay.

Flow in the saturated-unsaturated medium is posed and solved with a pressure head dependent variable The convection dispersion equation is amended to include retardation by adsorption and decay mechanisms. These continuum models are driven by complete physical properties and boundary condition information including: transient data for soil surface boundary conditions, hydraulic functions relating moisture content and hydraulic conductivity, and physical or chemical parameters (e.g., density, dispersivity, adsorption, and decay parameters).

CODE INPUT: Standard groundwater flow and contaminant transport parameters.

CODE OUTPUT: Predictions of head and concentration.

COMPILATION REQUIREMENTS: Predictions of head and concentration.

EXPERIENCE REQUIREMENTS: SUMATRA-I is written in FORTRAN IV. It consists of the main program and nine subprograms.

TIME REQUIREMENTS Extensive.

CODE VERIFICATION: Months.

DOCUMENTATION/REFERENCES:

van Genuchten, M.Th. (1978a) Mass transport in saturated-unsaturated media: one-dimensional solutions. Research Report 78-WR-11, Water Resources Program, Department of Civil Engineering, Princeton University, Princeton, NJ.

van Genuchten, M.Th. (1978b) Numerical solutions of the one-dimensional saturated-unsaturated flow equation. Research Report 78-WR-9, Water Resources Program, Department of Civil Engineering, Princeton University, Princeton, NJ.

SOURCE: SUMATRA-I was written by van Genuchten of the U.S. Salinity Laboratory. The code is in the public domain.

CODE NAME: SUTRA (Saturated-Unsaturated Transport)

PHYSICAL PROCESSES: Predicts fluid movement and the transport of either energy or dissolved substances in a subsurface environment.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite-element, and integrated finite-element.

DESCRIPTION: SUTRA flow simulation may be employed for areal and cross-sectional modeling of saturated groundwater flow systems, and for cross-sectional modeling of unsaturated zone flow. Solute transport simulation using SUTRA maybe employed to model natural or man-induced chemical species transport including processes of solute sorption, production, and decay, and may be applied to analyze groundwater contaminant transport problems and aquifer restoration designs. In addition, solute transport simulation with SUTRA may be used for modeling of variable density leachate movement and for cross-sectional modeling of salt-water intrusion in aquifers at near-well or regional scales, with either dispersed or relatively sharp transition zones between fresh water and salt water. SUTRA energy transport simulation may be employed to model thermal regimes in aquifers, subsurface heat conduction, aquifer thermal energy storage systems, geothermal reservoirs, thermal pollution of aquifers, and natural hydrogeological convection systems.

Mesh construction is quite flexible for arbitrary geometries employing quadrilateral finite elements in Cartesian or radial-cylindrical coordinate systems. The mesh may be coarsened employing "pinch nodes" in areas where transport is unimportant. Permeabilities may be anisotropic and may vary both in direction and magnitude throughout the system as may most other aquifer and fluid properties. Boundary conditions, sources, and sinks may be time-dependent. A number of input data checks are made in order to verify the input data set. An option is available for storing the intermediate results and restarting simulation at the intermediate time. An option to plot results produces output which may be contoured directly on the printer paper. Options are also available to print fluid velocities in the system and to make temporal observations at points in the system.

CODE INPUT: Standard groundwater flow and contaminant transport parameters.

CODE OUTPUT: SUTRA provides, as the primary calculated result, fluid pressures and either solute concentrations or temperatures, as they vary with time, everywhere in the simulated subsurface system.

COMPILATION REQUIREMENTS: SUTRA was written in FORTRAN 77.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Voss, C.I. A finite-element simulation model for saturated-unsaturated, fluid-density-dependent groundwater flow with energy transport or chemically-reactive single species solute transport. USGS Water Resources Investigations Report 84-4369.

SOURCE: The code was developed by C. I. Voss of the USGS Water Resources Department. The code is in the public domain.

CODE NAME: TRANUSAT

PHYSICAL PROCESSES: Predicts the transient migration of water and contamination in unsaturated and saturated geologic media.

DIMENSIONALITY: One and two dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The fundamental equations solved are the pressure head formulation of unsaturated water flow, Darcy's equation, and contaminant mass conservation. The principal assumptions are as follows:

- fluid flow is described by Darcy's equation;
- functional relationships exist for pressure head versus moisture content and hydraulic conductivity versus moisture content;
- solute transport may include advection, dispersion, diffusion, adsorption, and first-order reactions; and
- system properties may vary spatially.

CODE INPUT: Standard groundwater flow and contaminant transport parameters.

CODE OUTPUT: Predictions of head and concentration.

COMPILATION REQUIREMENTS: This one- and two-dimensional cartesian model includes the following boundary conditions:

- specified pressure head;
- specified fluid flux;
- specified concentration;
- zero concentration gradient;
- cauchy boundary condition; and
- boundary conditions may vary temporally.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Pickens, J.F.; Gillham, R.W.; Cameron, D.R. (1979) Finite-element analysis of the transport of water and solutes in tile-drained soils. Journal of Hydrology 40:243-264.

Pickens, J.F.; Gillham, R.W. (1980) Finite element analysis of solute transport under hysteretic unsaturated flow conditions." Water Resour. Res. 16(6):1071-1078.

SOURCE: TRANUSAT is a Geologic Testing Consultants, Ltd., proprietary code developed at GTC.

CODE NAME: TRUST

PHYSICAL PROCESSES: Predicts transient fluid movement in a multi-dimensional, partially saturated or saturated, deformable porous media.

DIMENSIONALITY: Multi-dimensional.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: TRUST is based on a volumetric expression of the continuity equation applied to a flow region of finite volume. The method of integral finite differences is used to represent the problem. Essentially, the model domain is a conglomeration of arbitrarily shaped volumes linked by connectors representing the porous media between volume nodal points. Changes in pressure at each node are computed for each time step by a finite-difference algorithm that uses both explicit (point-by-point) and implicit (simultaneous) solution schemes. Darcy velocities are calculated through finite-difference gradients of computed pressure heads.

It features the processes of:

- pore desaturation;
- hysteresis in permeability and saturation behavior;
- fluid compressibility; and
- one-dimensional (vertical) deformation of the soil skeleton due to water withdrawal.

The discretization of the continuity equation features a variable weighting scheme that allows the solution to range between central and backward differencing. The weighting factor is computed by TRUST at every time step based on the rate of pressure change. Slowly changing phenomena are weighted toward central differencing while rapid changes are weighted toward backward differencing. Regardless of the weighting scheme, the discretized equation contains both explicit and implicit parts. The explicit portion of the equation is used to solve for the pressure change over the entire domain. At locations where the explicit stability constraint for time step size is violated, the implicit part of the equation is applied and added to the existing explicit solution. Thus, the final matrix of equation coefficients created by the mixed explicit-implicit algorithm can be partitioned into those submatrices that require simultaneous solution.

The volumetric equation of mass conservation balances external fluxes and internal fluid generation with changes in mass storage. Nonlinearity in the formulation arises in the pressure-dependent permeability and fluid density in the external flux calculation, and pressure-dependent processes of fluid compressibility. Nonlinearity also arises from soil skeleton deformation and pore desaturation in the mass storage calculation. TRUST circumvents an iterative solution by using a point-slope prediction of pressure at the new time level to calculate the dependent parameters. Pressure is then solved with the nonlinear equation set.

TRUST uses an iterative overrelaxation matrix solver to compute the pressure changes at the new time level. For smaller matrices, iterative solvers are more efficient than direct solution techniques. However, convergence in highly nonlinear problems can be poor.

Selecting an appropriate time step is crucial to the success of the quasi-linearization approximation used in TRUST. For this reason, time step size is computed internally, based on the following criteria:

- the maximum pressure change is maintained at an average of a specified value;
- time- and pressure-dependent functions are not allowed to change more than an average of 1%; and
- convergence of the matrix solution must be satisfied in under 80 iterations.

Results of time steps that exceed any of these limits are discarded and the time step is halved.

Mass balance error in TRUST is monitored for each node and for the entire system being modeled. Model errors are discussed in the following categories:

- inaccurate specifications or interpolation;
- time truncation;
- pressure truncation;
- convergence; and
- machine roundoff.

Assumptions and simplifications for TRUST are:

- parameters can be functions of time, space, or pressure;
- hysteresis is modeled approximately by the use of scanning curves;
- fluid density, volume, void ratio, and saturation are functions of pressure only;
- flow region deforms with time;
- deformation of the media structure is one dimensional according to Terzaghi's theory of consolidation;
- for shallow reservoirs, deformation is expressed at the ground surface as subsidence;
- deep reservoirs with overburden are not resolved accurately by the consolidation computation;
- soil structure has a constant volume of incompressible solids;

- during the time interval, the elevation of the matrix is unchanged;
- time effects of consolidation are ignored;
- media properties are isotropic; and
- the model is best suited to soils of moderate to high saturation.

CODE INPUT: System properties required by TRUST are standard soil data usually included in a field sampling program:

- initial drying or wetting state;
- elevation to land surface from zero datum;
- average specific gravity of flow region material;
- fracture length or characteristic length;
- flow rate from well per unit aquifer thickness;
- permeability, analytical, or tabulated function of pressure;
- specific storage, analytical, or tabulated function of pressure;
- saturation, tabulation function of pressure;
- reference void ratio;
- reference effective stress;
- void ratio as a function of effective stress;
- deformability of matrix;
- swelling index;
- compression index; and
- slope of the void ratio versus log permeability relationship.

Fluid properties required by TRUST can be found in handbooks:

- viscosity;
- compressibility coefficient;
- density at atmospheric pressure; and
- gravitational constant.

Initial concentrations for TRUST are spatially distributed pressure heads and fluid generation rates. An application of the steady-state option of the model will generate a physically meaningful initial condition. Boundary conditions fall into three categories:

1) flux;

2) pressure head; and

3) flux or pressure head, when controlling conditions are unknown.

These boundary conditions can be constant, time-dependent, or sinusoidal. Flux boundary conditions occur at nodes with very small fluid mass capacity where a fixed or variable fluid generation rate is specified. These "artificial" nodes are then connected to the actual surface nodes of the problem. For fluid flux from the problem domain, external connectors with constant or tabulated functions of pressure or time are used to transfer fluid. Seepage faces are possible in TRUST with the assumptions of atmospheric pressure and one-way efflux.

The time-dependent boundary conditions can be input on a regional basis and can be incremented by a constant change. Regional input of parameter data is also available. Changes in the problem geometry can be done by using the model-scale factor to regionally reduce or measure the length scales of the original problem.

During execution, TRUST performs a check of the input data for consistency. Upon detection of an error, diagnostic statements are printed, which enable the user to trace and correct the mistake. The user's manual presents guidelines for the input of data tables and possible actions to correct inaccurate results.

CODE OUTPUT: TRUST has the following output results:

- input data echo
- input error summary
- results of the first, second, and last time steps are always printed
- system results
  - net fluid flow into system
  - average pressure change
  - average fluid flow rates
  - fluid mass capacity
  - moisture content
  - fluid generation rate
  - fluid generation amount
- levels of output to select from
  - fluid pressure
  - elevation
  - pressure change during time step
  - estimated time derivatives of pressure
  - fluid generation
  - total fluid content
  - change in fluid content
  - net fluid transported into node by internal and external information

- boundary information
  - pressure
  - net fluid flow into system from boundary node
  - average fluid flow rate
  - flow into node
  - flow rate across connection

- nodal
  - type
  - volume
  - density
  - fluid capacity
  - permeability
  - conductance from node, N
  - time constant
  - void ratio
  - saturation
  - preconsolidation stress

- connection
  - area
  - overall conductance
  - net fluid flow
  - average rate of fluid flow
  - flow into node
  - flow rate across a connection
  - fluid transfer coefficient (for external connection)

- diagnostics
  - flags node changing to a special node
  - nonconvergence
  - repeat of a time step due to criteria violation

The user has control over the frequency and level of detail for the output.

COMPILATION REQUIREMENTS: TRUST is written in FORTRAN with versions existing on the following computer systems:

- UNIVAC

- CDC 6400/6000/7000

- DEC VAX 11/780.

Single- and double-precision versions exist on the VAX. The double-precision version has an accuracy of eight byte words, which is standard on the UNIVAC and CDC machines. In addition, the VAX versions return run-time information to the terminal from which they are run.

Current problem limits are:

- 10 materials;

- 1 fluid property;

- 300 nodes;
- 600 internal connections;
- 20 external connections;
- 20 boundary nodes;
- 100 fluid generation tables;
- 300 initial conditions; and
- 100 table lengths.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS Months.

CODE VERIFICATION: TRUST has been verified against analytical solutions of flow problems, in particular:

- Theis solution for radial flow to a well; and
- Carslaw and Jaeger solution for a continuous point source in an isotropic three-dimensional medium.

Validation of the consolidation mechanism of the code has been performed in the following problem areas:

- saturated flow;
- unsaturated flow;
- saturated-unsaturated flow; and
- liquefaction.

Most of the validation tests are based on results observed with laboratory models, and encompass one-, two-, and three-dimensional problems on both rectangular and radial coordinate systems.

DOCUMENTATION/REFERENCES:

McKeon, T.J.; Tyler, S.W.; Mayer, D.W.; Reisenauer, A.E. (1983) TRUST-II utility package: partially saturated soil characterization, grid generation, and advective transport analysis. NUREG/CR-3443, U.S. Nuclear Regulatory Commission, Washington, DC.

Narasimhan, T.N. (1975) A unified numerical model for saturated- unsaturated groundwater flow. LBL-8862, Lawrence Berkeley Laboratory, Berkeley, CA.

Narasimhan. T.N.; Witherspoon, P.A. (1977) Numerical model for saturated-unsaturated flow in deformable porous media, 1. theory." Water Resour. Res. 13(3):657-664.

Narasimhan, T.N.; Witherspoon, P.A.; Edwards, A.L. (1978) Numerical model for saturated-unsaturated flow in deformable porous media, 2. The algorithm. Water Resour. Res. 14(2):255-261.

Narasimhan, T.N.; Witherspoon, P.A. (1978) Numerical model for saturated-unsaturated flow in deformable porous media, 3. Applications. Water Resour. Res. 14(6):1017-1034.

Reisenauer, A.E.; Key, K.T.; Narasimhan, T.N.; Nelson, R.W. (1982) TRUST: a computer program for variably saturated flow in multidimensional deformable media. PNL-3975, Pacific Northwest Laboratory, Richland, WA.

SOURCE: TRUST was developed by T. N. Narasimhan at the Lawrence Berkeley Laboratory. The code is in the public domain.

NUMERICAL SOLUTE TRANSPORT (SATURATED)

CODE NAME: CHAINT

PHYSICAL PROCESSES: Simulates the transport of radionuclides in a fractured porous medium.

DIMENSIONALITY: Two dimensional (x,y cartesian).

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The CHAINT model simulates multicomponent nuclide transport in a fractured-porous medium. The processes modeled include advection, dispersion/diffusion, sorption, chain decay coupling, and mass release. The computational method is based on a finite-element solution of the system of equations. Continuum portions of the medium are modeled as a single porosity system using two-dimensional isoparametric elements. Discrete fractures are modeled using isoparametric line elements embedded along the sides of the two-dimensional elements. Principal input to the code is the groundwater flow calculation obtained with the MAGNUM2D code (or a comparable nonisothermal flow model).

The principal assumptions of the code are:

- The diffusive flux Jri is assumed to be Fickian.
- Radionuclide transport occurs only in the fractures.
- Sorption may be represented by equilibrium adsorption.

In addition, the assumptions incorporated in MAGNUM2D must also be incorporated in CHAINT, these being:

- The fractured-porous medium is nondeformable.
- The fluid is slightly compressible.
- Flow is laminar (Darcian).
- Macroscale (REV) hydraulic gradients are independent of fracture orientation or geometry.
- The fluid system is single phase.
- The medium is fully saturated.
- Moisture is stored in both primary and secondary pores.
- Flow in fractures is governed by a nonisothermal version of Darcy's Law.
- Flow between primary and secondary pores depends on the difference between primary and secondary heads.
- Heat flux is governed by the convection-diffusion equation.

- Conservation of mass applies separately in the primary and secondary storage systems, but conservation of energy applies in the system as a whole.

CODE INPUT: As previously mentioned, principal input to the code is the groundwater flow calculation obtained with the MAGNUM2D code (or a comparable nonisothermal flow model). Other necessary inputs include:

- mesh geometry;
- half lives of the radionuclide contaminants;
- retardation factor of each contaminant;
- velocity field;
- mass dispersion tensor;
- nuclide splitting;
- decay constants;
- secondary porosity;
- mass source term;
- fluid density;
- initial parent concentrations; and
- initial daughter product concentrations

CODE OUTPUT: Output for CHAINT consists of the concentration of each radionuclide in the fractures at each time step.

COMPILATION REQUIREMENTS: Unknown.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The code CHAINT was tested against an analytical solution based on the uranium decay series. The code is in the public domain.

DOCUMENTATION/REFERENCES:

King, I.P.; McLaughlin, D.B.; Norton, W.R.; Baca, R.G.; Arnett, R.C. (1981) Parametric and sensitivity analysis of waste isolation in a basalt medium. Rockwell Hanford Operations Report RHO-BWI-C-94.

Baca, R.G.; Arnett, R.C.; King, I.P. (1981) Numerical modeling of flow and transport in a fractured-porous rock system. Rockwell Hanford Operations Report RHO-BWI-SA-113.

Neretnieks, I. (1980) Diffusion in the rock matrix: an important factor of radionuclide retardation? J. Geophys. Res. 84(B8):4379-4397.

SOURCE: CHAINT was developed by Resource Management Associates, Lafayette, California, for Rockwell Hanford Operations.

CODE NAME: DUGUID-REEVES

PHYSICAL PROCESSES: Predicts contaminant transport for use on the flow model results produced by the REEVES-DUGUID flow model.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: 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.

A special, rather standard numbering scheme for element nodes is used to reduce the matrix bandwidth that must be stored and operated upon for solution. Special treatment of various boundary condition is also used to maintain the desired matrix form. The actual solution is standard Gaussian elimination by decomposition into the product of 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.

CODE INPUT: Input for DUGUID-REEVES is the saturated/unsaturated flow model results from REEVES-DUGUID.

CODE OUTPUT: Predicts contaminant concentrations.

COMPILATION REQUIREMENTS: DUGUID-REEVES is written in FORTRAN and is operational on IBM systems.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Duguid, J.O.; Reeves, M. (1976) Material transport through porous media: a finite element Galerkin model. ORNL-4928, Oak Ridge National Laboratory, Oak Ridge, TN, March.

Reeves, M.; Duguid, J.O. (1975) Water movement through saturated-unsaturated porous media: a finite-element Galerkin model. ORNL-4927, Oak Ridge National Laboratory, Oak Ridge, TN.

SOURCE: The code was developed by J. O. Duguid of Battelle Memorial Institute and M. Reeves of Oak Ridge National Laboratory. The code is in the public domain.

CODE NAME: GROVE/GALERKIN

PHYSICAL PROCESSES: This model employs Galerkin finite-element methods to solve mass transport equations. The model successfully simulates solute transport for an unreactive conservative solute chloride, a solute with a first-order irreversible rate reaction, radioactive decay, and a solute with equilibrium controlled ion exchange.

DIMENSIONALITY: Three dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The partial differential equation that describes the transport and reaction of chemical solutes in porous media was solved using the Galerkin finite-element technique. These finite elements were superimposed over finite difference cells used to solve the flow equation. Both convective and flow due to hydraulic dispersion were considered. Linear and Hermite cubic approximations (basis functions) provided satisfactory results; however, the linear functions were found to be computationally more efficient for two-dimensional problems. Successive overrelaxation (SOR) and iteration techniques using Tchebyschef polynominals were used to solve the space matrices generated using the linear and Hermite cubic functions, respectively. Comparisons of the finite-element methods to the finite-difference models and to analytical results indicate that a high degree of accuracy may be obtained using the method outlined The technique was applied to a field problem involving an aquifer contaminated with chloride, tritium, and ^{90}Sr.

CODE INPUT: Unknown.

CODE OUTPUT: Unknown.

COMPILATION REQUIREMENTS: GROVE/GALERKIN is written in FORTRAN and is operational on an IBM 360 system.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Grove, D.B. The use of Galerkin finite-element methods to solve mass-transport equations. Water Resources Investigation 77-49, U.S. Geological Survey, Water Resources Division, Denver, CO.

SOURCE: This code is written by D. B. Grove of the U.S. Geological Survey, Water Resources Division. The code is in the public domain.

CODE NAME: ISOQUAD, ISOQUAD2

PHYSICAL PROCESSES: Predicts contaminant transport.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: This model uses 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.

CODE INPUT: Unknown.

CODE OUTPUT: Unknown.

COMPILATION REQUIREMENTS: ISOQUAD and ISOQUAD2 are written in FORTRAN and implemented on an IBM 360/91 machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Pinder, G.F. (1973) A Galerkin-finite-element simulation of groundwater contamination of Long Island, New York. Water Resour. Res. 9(6):1657-1669.

SOURCE: The codes were written by George Pinder of Princeton University and Emil Frind of the University of Waterloo. The code is in the public domain.

CODE NAME: KONBRED, USGS2D-MOC

PHYSICAL PROCESSES: KONBRED simulates groundwater flow and solute transport in one or two dimensions. Radioactive decay is not included in the program as originally published. A modified version has been prepared which incorporates decay of single species but omits formation of radioactive daughter products.

DIMENSIONALITY: One or two dimensional.

SOLUTION TECHNIQUE: Groundwater flow -- numerical, finite difference. Transport -- random walk.

DESCRIPTION: KONBRED solves the groundwater flow equation by a finite-difference method. It then computes solute transport in the calculated flow field by the method of characteristics. Both steady-state and transient flows can be calculated, and the aquifer may be heterogeneous and anisotropic. Forces resulting from differences in temperature or concentrations of dissolved solids are not considered.

Advective transport is computed by tracking particles, and a finite-difference method is used after each step to treat dispersion, fluid sources and sinks, and velocity divergence. The code can accommodate injection and withdrawal wells, diffuse leakage, and a variety of boundary and initial conditions. The modified version includes radioactive decay (but not formation of radioactive daughters) and equilibrium sorption. The code represents a two-dimensional area as a rectangular network of equally-spaced nodes. As presently written, there can be no more than 20 rows and 20 columns of nodes. The principle assumptions of the code include:

- Darcy's Law is valid and hydraulic-head gradients are the only significant driving mechanism for fluid flow.
- The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.
- Gradients of fluid density, viscosity, and temperature do not affect the velocity distribution.
- The two-dimensional solute transport equation is valid.
- Sorption may be represented as equilibrium adsorption.
- Vertical variations in head and concentration are negligible.
- The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

CODE INPUT: The principal inputs to the original versions are as follows:

- transmissivity tensor;
- aquifer thickness at each node;
- diffuse recharge and discharge at each node;

- initial head at each node;
- initial solute concentration at each node;
- storage coefficient;
- location of no-flow boundaries;
- effective porosity;
- longitudinal dispersivity;
- lateral dispersivity;
- locations of wells;
- pumping rate of each well;
- solute concentrations at each injection well; and
- pumping period.

The revised version requires additional inputs describing sorption and radioactive decay.

CODE OUTPUT: The principal output are the heads and concentrations. These can be printed out either after each time step at up to 5 "observation wells" or at all nodes after each 50 time steps.

COMPILATION REQUIREMENTS: The original program is written in FORTRAN IV and is compatible with many computers. It has been run successfully on Honeywell, IBM, DEC, Univac, and CDC computers. The revised program is written in FORTRAN 77 and, apparently, has run on IBM and CDC computers.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: KONBRED has been tested by comparison with several analytical solutions. Results from these comparisons are included in the documentation (ref. 1) and include both one-dimensional steady-state flow and plane radial steady-state flow.

This code (or earlier versions of it) has been applied to a wide variety of field problems. These include 1) chloride movement at the Rocky Mountain Arsenal (ref. 2); 2) chloride buildup in a stream-aquifer system (ref. 3); and 3) radionuclide transport at INEL (ref. 4).

DOCUMENTATION/REFERENCES:

Konikow, L.F.; Bredehoeft, J.D. (1978) Computer model of two-dimensional solute transport and dispersion in groundwater. Techniques of Water-Resources Investigations of the United States Geological Survey, Book 7, Chapter C2.

Konikow, L.F. (1977) Modeling chloride movement in the alluvial aquifer at the Rocky Mountain Arsenal, Colorado. U.S. Geological Survey Water-Supply Paper 2044.

Konikow, L.F.; Bredehoeft, J.D. (1974) Modeling flow and chemical quality changes in an irrigated stream-aquifer system. Water Resour. Res. 10(3):546-562.

Robertson, J.B. (1974) Digital modeling of radioactive and chemical waste transport in the Snake River plain aquifer at the National Reactor Testing Station, Idaho. U.S. Geological Survey Open-File Report IDO-22054.

Tracy, J.V. (1982) User's guide and documentation for adsorption and decay modifications to the U.S.G.S. solute transport model. U.S. Nuclear Regulatory Commission Report NUREG/CR-2502.

SOURCE: The model was developed by L. F. Konikow and J. D. Bredehoeft of the U.S. Geological Survey. The modifications were made by J. V. Tracy of ERTEC. The code is in the public domain.

CODE NAME: DPCT (Deterministic-Probabilistic Contaminant Transport)

PHYSICAL PROCESSES: Predicts groundwater flow and contaminant transport accounting for advection, dispersion, radioactive decay, and equilibrium sorption for a single contaminant.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Flow distribution -- numerical, finite element. Solute transport -- particle-tracking method.

DESCRIPTION: The code treats a two-dimensional vertical cross-section. Almost any water table and geologic configuration is permissible, and there are a variety of allowable boundary conditions. Water flow is steady state.

The cross section is divided into a rectangular array of cells. The head distribution is found by the finite-element method. Solute transport is then treated by tracking the motion of individual particles.

DPCT will calculate the long-term effects of a repository for specified scenarios, if used in conjunction with a biosphere transport code (e.g., PABLM). The code solves an inherently deterministic problem -- solute transport with known velocity and dispersion -- in a probabilistic manner. It does not treat any probabilistic problems.

The principal assumptions of the code are:

- A treatment in a two-dimensional cross section is acceptable.
- The solute transport equation is valid.
- Sorption may be represented as equilibrium adsorption with the distribution coefficient given by Equation 8.25.
- Principal axes of the transmissivity tensor are parallel to coordinate axes everywhere.
- Groundwater flows are steady state.

CODE INPUT: Inputs for DPCT include:

- hydraulic conductivity (horizontal and vertical) at each node;
- porosity at each node;
- longitudinal dispersivity at each node;
- ion exchange capacity at each node;
- location of water table;
- boundary conditions; and
- contaminant input rates and locations.

CODE OUTPUT: The principal outputs are maps of velocity or head and of contaminant concentration at any times selected by the user. A wide variety of other optional outputs are available.

COMPILATION REQUIREMENTS: The program is written in FORTRAN IV and has been run on an Amdahl 470V/7 computer. The code is in the public domain.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION:

DOCUMENTATION/REFERENCES:

Schwartz, F.W.; Crowe, A. (1980) A deterministic-probabilistic model for contaminant transport. U.S. Nuclear Regulatory Commission Report NUREG/CR-1609, August.

CGS, Inc. (1980) Scenario development and evaluation related to the risk assessment of high level radioactive waste repositories. U.S. Nuclear Regulatory Commission Report NUREG/CR-1608, August.

Schwartz, F.W. (1978) Application of probabilistic-deterministic modeling to problems of mass transport in groundwater system. Third International Hydrology Symposium, Ft. Collins, pp. 281-296.

Detailed derivations are given in:

Ahlstrom, S.W.; Foote, H.P.; Arnett, R.C.; Cole, C.R.; Serne, R.J. (1977) Multicomponent mass transport model: theory and numerical implementation (discrete-parcel-random walk version). Battelle, Pacific Northwest Laboratory Report PNL-2127.

SOURCE: DPCT was developed by Franklin Schwartz and A. Crowe of CGS, Inc.

CODE NAME: MMT (Multicomponent Mass Transport)

PHYSICAL PROCESSES: Predicts the transport profile of dissolved contaminants in groundwater.

DIMENSIONALITY: One dimensional.

SOLUTION TECHNIQUE: Discrete-parcel random-walk method.

DESCRIPTION: In the formulation of a mathematical model for simulating transport processes in the environment, the system of interest can be viewed as a continuum of matter and energy or as a large set of small discrete parcels of mass and energy. The latter approach is used to formulate the discrete-parcel random-walk transport model. Each parcel has associated with it a set of spatial coordinates, as well as a set of discrete quantities of mass and energy. A parcel's movement is assumed to be independent of any other parcel in the system. A Lagrangian scheme is used to compute the parcel advection, and a Markov random-walk concept is used to simulate the parcel diffusion and dispersion. The random-walk technique is not subject to numerical dispersion, and it can be applied to three-dimensional cases with only a linear increase in computation time. A wide variety of complex source-sink terms can be included in the model with relative ease. Examples of the model's application include the areas of oil spill drift forecasting, coastal power plant effluent analysis, and solute transport in groundwater systems.

The principal assumptions of the code are:

- The effect of changing atmospheric pressure is negligible
- Flow patterns are independent of the chemical composition or temperature of the groundwater solution.
- Hydrodynamic dispersion processes can be included with molecular diffusion.
- Relative mass flux can be adequately described by Fick's First Law.
- Darcy's Law holds for description of saturated groundwater flow.
- Total mass density of the mixture is constant.
- The number or type of particles does not significantly alter the flow properties of the host medium.
- The one-dimensional solute transport equation is valid.
- Sorption may be represented by equilibrium adsorption.

CODE INPUT: Inputs for MMT include:

- retardation coefficient;
- dispersion;

- half lives for all nuclides;
- path length;
- groundwater velocity;
- flow tube size;
- initial inventory;
- time after repository closure when the breach occurs;
- leach information to control entry of waste into groundwater system; and
- a mapping illustrating the parent-daughter relationships.

CODE OUTPUT: The principal outputs of MMT are the release rates of the contaminants. Both printed and graphic output are available and the output can be communicated to codes which calculate doses to humans.

COMPILATION REQUIREMENTS: MMT is written in FLECS, a higher-order language which compiles into FORTRAN, and is operational on a VAX machine. The code is in the public domain.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: MMT was compared to analytic results from GETOUT for a variety of problems.

DOCUMENTATION/REFERENCES:

Ahlstrom, S.W.; Foote, H.P.; Arnett, R.C.; Cole, C.R.; Serne, R.J. (1977) Multicomponent mass transport model: theory and numerical implementation (discrete-parcel-random-walk version). Pacific Northwest Laboratory Report BNWL-2127, May.

Washburn, J.F.; Kaszeta, F.E.; Simmons, C.S.; Cole, C.R. (1980) Multicomponent mass transport model: a model for simulating migration of radionuclides in groundwater. Pacific Northwest Laboratory Report PNL-3179, July.

SOURCE: MMT was developed at Battelle, Pacific Northwest Laboratories.

CODE NAME: PINDER

PHYSICAL PROCESSES: Predicts the movement of groundwater contaminants.

DIMENSIONALITY: Three dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The Galerkin method of approximation in conjunction with the finite-element method of analysis is used to simulate the movement of groundwater contaminants. In solving groundwater flow and mass transport equations, this approach allows a functional representation of the dispersion tensor, transmissivity tensor, and fluid velocity, as well as an accurate representation of boundaries of irregular geometry.

CODE INPUT: Unknown.

CODE OUTPUT: Unknown.

COMPILATION REQUIREMENTS: PINDER is written in FORTRAN and implemented on an IBM 360 or 390 machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: A field application of the method to chromium contamination on Long Island, New York, shows that accurate simulations can be obtained.

DOCUMENTATION/REFERENCES:

Pinder, G.F. (1973) A Galerkin-finite element simulation of groundwater contamination on Long Island, New York. Water Resour. Res. 9(6):1657-1669.

SOURCE: PINDER was developed by G. F. Pinder at Princeton University. The code is in the public domain.

CODE NAME: ROBERTSON1

PHYSICAL PROCESSES: Predicts the movement of radionuclides by groundwater and soil transport.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Analytical and numerical, finite difference.

DESCRIPTION: Aqueous chemical and low-level radioactive effluents have been disposed to seepage ponds since 1952 at the Idaho National Engineering Laboratory. The solutions percolate toward the Snake River Plain aquifer (9,135 m below) through interlayered basalts and unconsolidated sediments and an extensive zone of groundwater perched on a sedimentary layer about 40 m beneath the ponds. A three-segment numerical model was developed to simulate the system, including effects of convectional hydrodynamic dispersion, radioactive decay, and adsorption. The first segment uses an analytical solution to simulate transport from the ponds to the 25-m thick perched water lens, assuming steady vertical flow through a 15-m long saturated homogeneous column. The second segment simulates two-dimensional horizontal transport in the perched water body using finite-difference methods, assuming complete vertical mixing with vertical leakage from the bottom. The third segment simulates simulates vertical solute transport from the perched water body toward the aquifer by assuming unsaturated, but steady water flow in a series of contiguous, nonhomogeneous independent vertical columns. The transport equation is solved by a "hop-scotch" finite-difference scheme for each column. Simulated hydraulics and solute migration patterns for all segments agree adequately with the available field data. The model can be used to project subsurface distributions of waste solutes under a variety of assumed conditions for the future.

CODE INPUT: Standard hydrologic and transport parameters.

CODE OUTPUT: Predicts head and concentration.

COMPILATION REQUIREMENTS: ROBERTSON1 is written in FORTRAN and implemented on a CDC machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The code has been verified by the Idaho site application.

DOCUMENTATION/REFERENCES:

Robertson, J.B. (1974) Digital modeling of radioactive and chemical waste transport in the Snake River plain aquifer at the National Reactor Testing Station, Idaho. U.S. Geological Survey Open-File Report, AEC No. IDO-22054, 41 pp.

SOURCE: ROBERTSON1 was developed by J. B. Robertson of the U.S. Geological Survey, National Center. The code is in the public domain.

CODE NAME: ROBERTSON2

PHYSICAL PROCESSES: Predicts groundwater transport of radioisotopes.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite-difference, and method-of-characteristics solution technique.

DESCRIPTION: ROBERTSON2 was developed to predict radioisotope migration at the National Reactor Testing Station. The influences on migration include space and time variations in groundwater flow, hydraulic dispersion, radioactive decay, ion exchange, and other chemical reactions. These processes are included in problems of movement of radioactive wastes in groundwater; design and analysis of tracer tests in groundwater systems; and analysis of natural isotope distributions in groundwater. The model is composed of two coupled phases: the first simulates the hydraulics, and the second simulates solute transport. The hydraulic phase solves the transient, two-dimensional, partial-differential equation of groundwater flow for a bounded, two-dimensional, one-layer aquifer, using finite-difference techniques (iterative, alternating direction, implicit scheme). This method is described by Bredehoeft and Pinder. Groundwater velocity vectors are computed by this equation, for every grid point at any finite time step. The velocities are transferred to the solute transport phase of the model that solves the transient particle differential equation of the transport, using the method of characteristics. The method characterizes the dissolved nuclides by characteristic imaginary particle. Considered terms of the solute transport phase are: hydraulic dispersion, convective transport, aquifer compression factors, sources and sinks, radioactive decay, and sorption.

CODE INPUT: Input for the model includes transmissivity, storage coefficient, boundaries, hydraulic dispersion coefficients (transverse and longitudinal), initial concentration distributions, ion exchange, distribution coefficient, radioactive decay constant, and source-sink inputs.

CODE OUTPUT: Predicts head and concentration.

COMPILATION REQUIREMENTS: ROBERTSON2 is written in FORTRAN and implemented on a CDC machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Bredehoeft, J.D.; Pinder, G.F. (1973) Mass transport in flowing groundwater. Water Resour. Res. 9(1):194-210.

SOURCE: ROBERTSON2 was developed by J. B. Robertson of the U.S. Geological Survey, National Center. The code is in the public domain.

CODE NAME: SWENT

PHYSICAL PROCESSES: Predicts fluid, energy, and solute radionuclide transport.

DIMENSIONALITY: One dimensional, two dimensional, axisymmetric (r-z), and three dimensional.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: SWENT is based on the coupled, transport solution of the fluid, energy, and solute transport equations. Fluid density and viscosity in this code are treated as functions of pressure, temperature, and solute concentration; thus, the transport equation set being solved is nonlinear. SWENT can be applied in one-dimensional, two-dimensional (x-y, x-z), axisymmetric (r-z), and three-dimensional (x-y-z) heterogeneous geologic systems. The code also features a comprehensive radionuclide transport model that includes a radionuclide data base and the ability to account for the generation and transport of daughter products in straight or branched decay chains. The user has the option to solve for any or all of the dependent variables. Basic processes addressed by SWENT include:

- confined flow of a two-component, single-phase fluid;
- pressure-dependent aquifer porosity;
- vertical recharge;
- detailed well-bore modeling based on well characteristics;
- convective and conductive heat transport;
- solute advection;
- hydrodynamic dispersion;
- first-order decay reactions;
- equilibrium isothermal sorption; and
- salt dissolution.

SWENT has an aquifer reservoir model that is coupled to a well-bore model. The well-bore model offers a more detailed account of the well-bore physics than is possible with the finite difference mesh of the general problem. Results from the modeling of the well are then applied as boundary conditions to the aquifer reservoir. The radionuclide modeling is not coupled to the flow, energy, and solute computations; consequently, this part of the simulation is performed independently after the pressure field has been established.

SWENT has an option that allows the effect of the surrounding aquifer to be incorporated into the aquifer boundary conditions without actually modeling the regional problem. Aquifer influence functions allow subregional modeling by posing boundary conditions that respond as if a larger aquifer were being modeled. Generally, these influence functions are necessary when the

simulation time is long enough for calculated changes to occur at peripheral grid blocks.

The well-bore model uses a direct simultaneous solution of the energy equation to calculate the pressure and temperature changes over the well-bore depth. On the other hand, the reservoir model is based on a semi-implicit finite-difference scheme of the flow, energy, and solute equations. The dependent variables in this formulation, pressure, temperature, and concentration appear in the space derivatives at the new time level.

An iterative procedure is used for the problem solution. Changes in the pressure, temperature, and concentration are computed by applying each equation sequentially with updated values for all dependent variables. Transmissibilities and dispersion, on the contrary, are always treated at the old iterate level. The iterative procedure ceases when the fractional density change falls below an internal tolerance.

Solution of the simultaneous equation is performed by a direct, reduced-band Gaussian elimination technique or an iterative, two-line, successive, overrelaxation method. Each method has an optimal range of applicability which is presented in the model documentation.

The principal assumptions of the SWENT code are:

- only a single-phase fluid exists;
- porous medium is saturated with fluid;
- flow is laminar and governed by Darcy's Law;
- kinetic energy is negligible in the energy balance;
- fluid viscosity is an exponential function of temperature, or a power law function of concentration;
- salt dissolution is a first-order reaction;
- linear equilibrium, sorption;
- hydrodynamic dispersion is a linear function of velocity; and
- effects of hydrodynamic dispersion and molecular diffusivity are additive.

CODE INPUT: The input requirements of SWENT are as follows:

- fluid compressibility;
- rock compressibility;
- fluid thermal expansion factor;
- heat capacity of rock;
- resident and injection fluid densities;

- resident and injection fluid viscosities;
- thermal conductivity of porous medium;
- hydrodynamic dispersivities;
- molecular diffusivity;
- porosity;
- hydraulic conductivity;
- well data
  - depth
  - diameter
  - roughness
  - heat transfer coefficient
  - pressure conditions; and
- adsorption distribution coefficient.

The specified boundary conditions of SWENT are as follows:

- constant pressure, temperature, concentration (Dirichlet);
- radiation boundary condition (Cauchy);
- steady-state or transient aquifer influence functions;
- heat loss to overburden and underburden;
- well specification of pressure, temperature; and concentration;
- radioactive sources; and
- recharge.

SWENT has many features that reduce the tedium of data entry: 1) grid-block characteristics can be entered on a regional basis; 2) boundary conditions are entered only when an update occurs; 3) any system of units can be used with the proper entry of conversion factors; 4) variable timestepping can be performed by a user-defined function; and 5) inclusion of a radionuclide data library. There is an input data checker in SWENT that alerts the user to up to 69 error conditions.

CODE OUTPUT: SWENT produces a very readable line printer output of computed results. The detail and frequency of the output is at the option of the user. Specifically, the available output include:

- input data echo;
- Darcy velocities;
- flow, heat, diffusive transmissibilities; viscosity, enthalpy, dispersivities; thermal conductivities in all grid blocks;

- fluid, energy, component, and nuclide balance;
- maximum pressure, temperature, concentration changes, and the corresponding grid blocks;
- well performance summary (pressure, concentration, temperature) at well head and bottom hole, and water, heat, and inert component production rates and their integrated values over time;
- aquifer influx rates for water, heat, and inert components;
- nuclide discharge rates at biosphere grid blocks;
- integrated nuclide discharge rates to different regions;
- pressure, temperature, component concentrations, and nuclide concentrations at all grid blocks;
- two-dimensional areal contour maps for pressure, temperature, brine, concentration, and nuclide concentration; and
- plots of pressure, temperature, and brine concentration for observed and calculated values at wells.

COMPILATION REQUIREMENTS: SWENT is written in FORTRAN with versions existing on the following computer systems:

- CDC 7600; and
- DEC VAX 11/780.

The code was designed to be executed on a CDC 7600 and includes external references to CDC-specific functions Conversion to the VAX 11/780 was hampered by these references. The VAX version of the code has dispensed with the dynamic allocation of core storage available on CDC hardware and replaced other CDC routines with function subroutines coded into the software. To equal the level of accuracy and range of the CDC 7600, real variables in the code were double-precisioned from four- to eight-byte decimal words with an extended range option.

Current limits to the code are:

- 20 wells;
- 7 overburden layers;
- 7 underburden layers;
- 50 aquifer influence functions; and
- 10 entries in the viscosity and temperature tables.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: SWENT has been verified against analytical solutions of fluid flow, heat flow, inert component transport, and radionuclide transport. Good agreement between model results and analytical solutions was found in each of the 11 cases cited. Three field applications of SWENT are included in the code documentation. The predicted SWENT results are in reasonable agreement with field observations.

DOCUMENTATION/REFERENCES:

INTERA Environmental Consultants, Inc. (1983) SWENT: a three- dimensional finite-difference code for the simulation of fluids, energy, and solute radionuclide transport. ONWI-457, Prepared for Battelle Memorial Institute, Office of Nuclear Waste Isolation, Columbus, OH.

SOURCE: SWENT was developed by S. B. Pahwa, R. B. Lantz, and B. S. Ramaro of INTERA Environmental Consultants, Inc.

CODE NAME: TRANS

PHYSICAL PROCESSES: Predicts groundwater pollution problems.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Random walk.

DESCRIPTION: TRANS provides a generalized computer code that can simulate a large class of problems involving convection and dispersion of chemical contaminants associated with fertilizer applications, hazardous waste leachate from landfilled and other sources, and injection of chemical waste into the subsurface using disposal wells. TRANS does not address density-induced convection. Concentration distribution in the aquifer represents a vertically-averaged value over the saturated thickness of the aquifer.

TRANS is capable of considering:

- Saturated groundwater flow in a single confined or unconfined aquifer where water flow is typically horizontal. (The code addresses temporal variations in two-dimensional (x-y) flow for a variety of boundary conditions and arbitrary x-y geometry.)
- Advection of a chemical contaminant in a saturated groundwater system released from a variety of typical sources.
- Hydrodynamic dispersion (both lateral and transverse) and diffusion of a chemical contaminant in a saturated groundwater system.
- Retardation of a chemical contaminant when it can be characterized by a constant Kd and the assumptions of instantaneous and reversible adsorption are adequate.
- Radioactive decay of a chemical contaminant.

TRANS addresses only a single aquifer. Spatial and temporal distribution of head in the aquifer can be calculated by four methods:

1) analytic (HSOLV2) solution for a uniform 1-ft/d flow in the x direction;

2) analytic (HSOLV4) solution to the Theis formula centered at node (15, 15);

3) numerical finite difference solution (HSOLVE) to the two-dimensional (x-y) vertically-averaged groundwater flow equation* (this solution is for transient or steady-state flow); and

4) user-supplied subroutine for reading or calculating head on the finite-difference grid used in the TRANS transport model.

The transport model portion of TRANS uses a direct simulation technique. The concentration of a chemical constituent in a groundwater system is assumed to be represented by a finite number of discrete particles. Each of these particles is moved according to the advective velocity and dispersed according to random-walk theory. The mass assigned to each particle represents a fraction of the total mass of chemical constituents involved. In the limit, as

the number of particle approaches the molecular level, an exact solution to the actual situation is obtained. This kind of transport model is inherently mass conservative. Convergence can be checked by increasing the number of particles. There are restrictions, as with any numerical method, which limit the size of time step that can be taken for both a time-dependent and spatially-dependent problem. Time steps for particles are limited such that advective plus dispersive movement is no greater than the spacing between velocity (head) nodes.

The principal assumptions regarding flow are:

- Darcian flow is assumed;
- flow in the aquifer is horizontal and controlled only by hydraulic head gradients;
- leakage between the simulated aquifer, rivers, lakes, other aquifers, and springs is a linear function of head difference with the slope of this relationship determined from the leakage parameter, K/m, where K is the permeability of the aquitard (or stream bed) and m is the thickness; and
- storage in the stream, lake, or river beds and aquitards is ignored.

The principal assumptions regarding contaminant transport are:

- the advection-diffusion equation for solute transport is assumed valid;
- dispersion in porous media is random process; and
- retention of a contaminant (or retardation of a concentration front) may be represented by an instantaneous and reversible sorption process.

CODE INPUT: Input requirements for the code are those typically available from standard field or laboratory measurements. For the flow portion of the model they include:

- a variable finite-difference grid description;
- time step and number of time steps to be run;
- areal distributions of
  - permeability
  - source aquifer potential for leaky artesian simulations
  - aquifer bottom elevations;
  - aquifer top elevations;
  - head (initial conditions)
  - aquitard thickness and permeability for leaky artesian aquifers
  - simulations
  - artesian and water table storage coefficients;
- pumping and recharge well locations and temporal rates;
- stream (river or lake) node locations, surface-water elevations, stream or lake bed thickness and permeability; fraction of node area available for transfer;

- constant head node locations and elevation for held head;
- location of springs, elevation at which spring flow begins, and slope of the spring flow versus groundwater head for the spring production line; and
- locations of nodes where evapotranspiration from the water table is to be considered and the slope of the rate versus head line and the water-table elevation at which evapotranspiration effects are to be ignored.

For the transport model, additional input requirements include:

- longitudinal dispersivity;
- lateral dispersivity;
- effective porosity;
- retardation factor or Kd;
- bulk mass density of porous medium;
- location and concentration of sources, description of source geometry, and selection of method for release of particles; and
- sink locations and groupings of sink locations for summarizing outflow versus time results.

The model contains no checking of input for consistency and automatic termination for faulty or inconsistent inputs.

CODE OUTPUT: Results are printed in a 132-character format with a concise and readable output layout. The code echoes input parameters and produces line printer plots of head, numbers of particles, and concentrations. The code also reports the concentration of water entering sink nodes and groups of sink nodes versus time. The code produces no contour maps or output fields that can be passed on to other computer system programs for plotting and produces no mass balance summaries for water flow or transport.

COMPILATION REQUIREMENTS: The TRANS code is written in FORTRAN and run on a CDC CYBER-175 machine. The code has also been brought up on a Digital Equipment Corporation VAX 11/780.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The code has been compared to analytic and hand-calculated examples.

DOCUMENTATION/REFERENCES:

McDonald, M.G.; Fleck, W.B. (1978) Model analysis of the impact on groundwater conditions of the Muskegon County waste-water disposal system, Michigan. U.S. Geological Survey Open-File Report 78-79.

Prickett, T.A.; Lonnquist, C.G. (1971) Selected Digital Computer techniques for groundwater resource evaluation. Illinois State Water Survey Bulletin 55.

Prickett, T.A.; Namik, T.G.; Lonnquist, C.S. (1981) A random-walk solute transport model for selected groundwater quality evaluations. Illinois State Water Survey Bulletin 65.

SOURCE: The program was written by Thomas A. Prickett of Thomas A. Prickett and Associates, and Thomas G. Naymik and Carl G. Lonnquist of Illinois Water Survey.

CODE NAME: TRANSAT2

PHYSICAL PROCESSES: Predicts groundwater flow and contaminant transport in saturated geologic media.

DIMENSIONALITY: Multi-dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: The fundamental equations solved are those of fluid mass conservation, Darcy's equation, and contaminant mass conservation. The principal assumptions are as follows:

- fluid flow may be described by Darcy's equation;
- steady-state groundwater flow exists;
- solute transport includes advection, dispersion, diffusion, adsorption, and first-order reactions (i.e., radioactive decay); and
- system properties may vary spatially.

TRANSAT2 utilizes the Galerkin finite-element technique with linear triangular elements. The solution technique is a Gaussian elimination method. This multi-dimensional code includes the following boundary conditions:

- specified hydraulic head;
- specified fluid flux;
- zero concentration gradient;
- cauchy boundary condition; and
- temporally varying solute boundary conditions.

CODE INPUT: Standard groundwater flow and contaminant transport.

CODE OUTPUT: Predicts head and concentration.

COMPILATION REQUIREMENTS: Unknown.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Pickens, J.F.; Lennox, W.C. (1976) Numerical simulation of waste movement in steady ground-water flow systems. Water Resour. Res. 12(2):171-180.

Lee, D.R.; Cherry, J.A.; Pickens, J.F. (1980) Groundwater transport of a salt tracer through a sandy lake bed. Limnology and Oceanography 25(1):45-61.

Grisak, G.E.; Pickens, J.F. (1980) Solute transport through fractured media -- I. the effect of matrix diffusion. Water Resour. Res. 26(4):719-730.

SOURCE: TRANSAT2 is a GTC proprietary code developed at Geologic Testing Consultants in Ottawa, Ontario, Canada.

NUMERICAL COUPLED CODES
(SOLUTE AND HEAT TRANSPORT)

CODE NAME: CFEST -- Coupled Fluid, Energy and Solute Transport

PHYSICAL PROCESSES: Fluid, energy, and solute transport in a confined, saturated aquifer.

DIMENSIONALITY: Up to three dimensional.

SOLUTION TECHNIQUE: Finite element.

DESCRIPTION: CFEST was developed for the analysis of a confined aquifer's response to thermal energy storage. This model employs a standard Galerkin finite-element method in the solution of the coupled equations of mass, energy, and solute-mass conservation. A sequential solution algorithm bearing resemblance to the SWIP model is used to solve the flow of water, the transport of energy, and finally the transport of solute. The finite-element approximation to the continuum is made with a bilinear, two-dimensional, quadrilateral element that is simply expanded to the trilinear, eight-node brick when three-dimensional analysis is warranted. CFEST can be used to analyze two-dimensional vertical or horizontal planes, two-dimensional axisymmetric cross sections, and fully three-dimensional aquifer situations. Verifications against analytical and semianalytical solutions have been made and are given in documentation on the model. CFEST has been applied to the analysis of solid waste landfills for the U.S. Environmental Protection Agency.

CFEST simulates confined, saturated aquifer systems. Unconfined, saturated aquifers can be simulated by assuming the top elevation of the aquifer is at the water table and assigning piezometric heads based on the water table elevation.

CODE INPUT: Finite-element grid describing soil profile geometry (two or three dimensional), soil hydraulic characteristics, recharge, solute characteristics (Kds), and time step size.

CODE OUTPUT: Output consists of line-print listings (output data files) and plots (output plot files) of potentials, temperatures, and solute concentrations at user-specified nodes (grid points).

COMPILATION REQUIREMENTS: CFEST is available in FORTRAN and is currently being used on DEC VAX 11/780 and MICRO-VAXs.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: CFEST has been verified against analytical and semianalytical solutions. Results of the verification are included in the model documentation.

DOCUMENTATION/REFERENCES:

Gupta, S.K.; Kincaid, C.T.; Meyer, P.R.; Newbill, C.A.; Cole, C.R. (1982) A multidimensional finite element code for the analysis of coupled fluid, energy, and solute transport (CFEST). PNL-4260, Pacific Northwest Laboratory, Richland, WA.

SOURCE:

S. K. Gupta
Office of Nuclear Waste Isolation
Battelle Memorial Institute
505 King Avenue
Columbus, OH 43201

C. T. Kincaid or C. R. Cole
Battelle, Pacific Northwest Laboratory
Battelle Boulevard
Richland, WA 99352

CODE NAME: GWTHERM

PHYSICAL PROCESSES: Predicts fluid flow and transport in a heated porous medium.

DIMENSIONALITY: Two dimensional.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: GWTHERM is a two-dimensional model based on the equations for nonisothermal single-phase flow and solute transport in porous media. It allows for anisotropy of hydraulic conductivities and inhomogeneous density and temperature-dependent fluid properties, and it uses the alternating-direction implicit technique with an integrated finite difference scheme to provide an unconditionally stable solution procedure. Recent development has coupled GWTHERM to DAMSWEL to include dependence of permeability on effective stress changes. In this sense the connection between these models is sequential rather than fully coupled, but it represents a capability available only in a code like STEALTH/HART.

CODE INPUT: Unknown.

CODE OUTPUT: Unknown.

COMPILATION REQUIREMENTS: GWTHERM is written in FORTRAN and implemented on a CDD 6600 system.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Runchal, A.;Treger, D.; Segal, G. (1979) Program EP21 GWTHERM: two-dimensional fluid flow, heat and mass transport in porous media. ATG/TN-LA-34, Advanced Technology Group, Los Angeles, CA, April.

SOURCE: GWTHERM was developed by A. Runchal of Dames & Moore's Advanced Technology Group. The code is in the public domain.

CODE NAME: OGRE

PHYSICAL PROCESSES: Predicts groundwater flow and nuclide transport in a heated porous medium.

DIMENSIONALITY: One or two dimensional.

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: OGRE can be used for the time simulation of fluid flow and mass transport through porous media, using an implicit (backward Euler) finite-difference scheme. Specifically, OGRE has been used to simulate the time-dependent flow of groundwater into or out of underground openings and the mass transport of radionuclides under the influence of a pressure gradient.

Parameters may be either time and space dependent or fixed in either time or space. Initial and boundary conditions may also vary with time and space. Zoning of the grid must be constant in both directions, but zoning is dynamic and set at execution time.

CODE INPUT: Unknown.

CODE OUTPUT: Unknown.

COMPILATION REQUIREMENTS: OGRE is written in FORTRAN and implemented on a CDC 7600 machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

Korver, J.A. (1970) UCRL-50820, Lawrence Livermore Laboratory, Livermore, CA, February.

SOURCE: OGRE was written by J. A. Korver of the Lawrence Livermore Laboratory. The code is in the public domain.

CODE NAME: SHALT (Solute, Heat, and Liquid Transport)

PHYSICAL PROCESSES: Predicts liquid flow, heat transport, and solute transport in a regional groundwater flow system.

DIMENSIONALITY: Two dimensional (x-y or x-z cartesian).

SOLUTION TECHNIQUE: Numerical, finite element.

DESCRIPTION: SHALT performs the two-dimensional simulation of fluid flow, solute transport, and heat transport in a porous medium. The spatial domain is discretized using three-noded triangular elements and the time domain by a fully implicit backward difference scheme. The aquifer parameters may be distributed or zoned and the system may be anisotropic. The viscosity of the liquid phase and the diffusion coefficient of the solute are functions of temperature. The density of the liquid phase is represented as a function of temperature and total solute concentration. The equations describing the fluid flow, energy transport, and solute transport are fully coupled with the dependent parameters upgraded after each time step. Fractured media may be modeled by treating the fractured rock as a continuum.

SHALT may be considered both a near-field and far-field code as temperature-dependent parameters have been implemented in this code. It would be considered more as a far-field code, however, as deformation and the stress/strain relationships are not considered in this model.

The main assumptions of the code are:

- Darcy's Law is valid;
- the compressibility and heat capacity of the liquid phase are constant;
- k, , o, and QP can vary spatially but do not vary with time and are not dependent on the concentration or the temperature;
- the thermal dispersion tensor for the liquid phase includes the effects of mechanical dispersion and thermal conduction and is a function of velocity;
- the exchange of heat and solute is instantaneous between the liquid and solid phases at the same point; and
- the hydrodynamic dispersion tensor for the liquid phases includes the effects of mechanical dispersion and thermal conduction and is a function of velocity.

CODE INPUT: Inputs to SHALT include:

- mesh geometry;
- initial heads;
- initial concentrations and initial temperatures;
- fluid density;

- porosity;
- compressibility of the fluid and porous medium;
- the permeability tensor;
- viscosity;
- solute density;
- heat capacity of both the solid and liquid phases;
- the thermal conductivity tensor;
- the thermal dispersivity tensor;
- the hydrodynamic dispersivity tensor;
- the first-order reaction constant;
- distribution coefficient; and
- the bulk density.

CODE OUTPUT: The output of SHALT consists of the pressure, concentration, and temperature distribution at each time step.

COMPILATION REQUIREMENTS: SHALT is written in FORTRAN IV.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: The liquid flow portion of the model was tested by calculating steady-state pressure and hydraulic head distributions for various flux inputs. Values of system parameters were chosen to be constant. The calculated hydraulic head gradient for steady-state conditions was correct.

The heat transport portion of the model was tested by comparison with results of the analytical solution of Bredehoeft and Papadopulos (ref. 2) for one-dimensional steady-state transport.

The solute transport portion of the model was tested by comparison with results of the analytical solution by Ogata and Banks (ref. 3) for one-dimensional advection-dispersion with a step input in concentration.

SHALT was used successfully to model results of pressure testing in fractured rock at Chalk River (ref. 4).

DOCUMENTATION/REFERENCES:

Pickens, J.F.; Grisak, G.E. (1979) Finite element analysis of liquid flow, heat transport, and solute transport in a ground-water flow system: governing equations and model formulation. Atomic Energy of Canada, Ltd., Report TR-81, September.

Bredehoeft, J.D.; Papadopulos, S.S. (1965) Rates of vertical groundwater movement estimated from the earth's thermal profile. Water Resour. Res. 1(2):325-328.

Ogata, A.; Banks, R.B. (1961) A solution of the differential equation of longitudinal dispersion in porous media. U.S. Geological Survey Professional Paper 411-A.

Davison, C.C. (1981) Physical hydrogeologic measurements in fractured crystalline rock: summary of 1979 research program at WNRE and CRNL. Atomic Energy of Canada, Ltd., Technical Record 161.

SOURCE: SHALT was developed by J. F. Pickens and G. E. Grisak of the Inland Waters Directorate, Environment Canada for Atomic Energy of Canada, Ltd. The code is in the public domain.

CODE NAME: SWIFT (Sandia Waste Isolation Flow and Transport)

PHYSICAL PROCESSES: Predicts flow, solute, and heat migration from the repository through the groundwater system.

DIMENSIONALITY: The pressure, temperature, and concentration field is represented by a series of three-dimensional rectangular cartesian grid points. In addition, a two-dimensional (r,z) grid system is also provided.

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: The code simulates the flow and transport of energy, solute, and radionuclides in a geologic media. SWIFT is a three-dimensional, finite-difference, groundwater flow and nuclide transport code. The model takes into account saturated flow in an isothermal or heated porous medium as well as sorption and desorption mechanisms. In addition, the code takes into explicit account nuclide decay and the creation of daughter products. For the nuclide decays, the code considers conservation of dissolved contaminants, energy, and total liquid mass. The fluid density can be a function of pressure, temperature, and concentration. Viscosity can also be a function of temperature and concentration. Aquifer properties can vary spatially. Hydrodynamic dispersion is described as a function of velocity. Boundary conditions allow natural water movement in the aquifer, heat losses to the adjacent formation and location of injection, production, and observation points anywhere in the system.

SWIFT solves four coupled differential equations, together with a number of submodels describing the nonlinearities, in a sequential manner. Options include:

- steady-state or transient flow;
- solute transport;
- eat transport;
- well bore;
- heterogeneous and/or anisotropic media;
- confined and/or water table conditions; and
- recharge and/or wells.

SWIFT is a descendant of the code SWIP (Survey Waste Injection Program, ref. 3) developed for the U.S. Geological Survey. SWIP was originally put together, in part, from oil industry codes.

The main assumptions of the code are:

- Flow follows Darcy's Law.

- Fluid density can be a function of pressure, temperature, and concentration of the inert component. Fluid viscosity can be a function of temperature and concentration.
- Injection wastes are miscible with the in-place fluids.
- Aquifer properties vary with position (i.e., porosity, permeability, thickness, and elevation can be specified for each grid block in the model).
- Hydrodynamic dispersion is described as a function of fluid velocity.
- Radioactive constituents are present in trace quantities only, that is, fluid properties are independent of the concentrations of these contaminants.
- The energy equation can be described as "enthalpy in - enthalpy out = change in internal energy of the system." This is rigorous except for kinetic and potential energy which have been neglected.
- Boundary conditions allow natural water movement in the aquifer, heat losses to the adjacent formations, and the location of injection, production, and observation points anywhere within the system.

CODE INPUT: Inputs for SWIFT include:

- half-life of each nuclide;
- distribution coefficient of each nuclide on each rock type;
- fluid compressibility;
- porous medium compressibility;
- coefficient of thermal expansion of fluid;
- fluid heat capacity;
- rock heat capacity;
- thermal conductivity of rock-fluid mixture in each direction for each rock type;
- longitudinal and transverse dispersivities for each rock type;
- molecular diffusivity in porous medium;
- rock density;
- fluid density;
- pressure and temperature of injected or produced fluids in each well;
- thermal diffusivity of rock surrounding well bores;

- fluid viscosity as a function of temperature and brine concentration;
- hydraulic conductivity of each rock type in each direction;
- porosity of each rock type;
- heat capacity of each rock type;
- boundary conditions;
- initial velocities and concentrations;
- salt dissolution rate in each rock type;
- size, placement, and contents of waste canisters;
- solubility limits;
- production rate of each well;
- location, angle, and depth of each well;
- diameter and pipe roughness of each well; and
- leaching time of wastes.

CODE OUTPUT: Output for SWIFT consists of the pressure, temperature, solute concentration, and the concentration of each radioactive isotope. These are given at every grid point after each time step as required.

COMPILATION REQUIREMENTS: SWIFT is written in FORTRAN IV for use on a CDC 6600 machine. With minor modifications, it can be used on other machines. This modification primarily involves the real-time dimensioning feature of SWIFT.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: To evaluate the effect of numerical truncation errors arising due to isotope decay terms and to develop a set of criteria to delete components in numerical simulations without losing any accuracy in the results, SWIFT was compared against the results from ORIGEN (ref. 2). The ORIGEN model is a matrix exponential solution of the Bateman equations for radioactive decay. The comparison was considered excellent. Other parts of SWIFT that solve for flow and transport have been tested against both analytical and laboratory results.

DOCUMENTATION/REFERENCES:

Dillon, R.T.; Lantz, R.B.; Pahwa, S.B. (1978) Risk methodology for geologic disposal of radioactive waste: the Sandia waste isolation flow and transport (SWIFT) model. Sandia National Laboratories Report SAND 78-1267.

Bell, M.J. (1973) ORIGEN -- the ORNL isotope generation and depletion code. Oak Ridge National Laboratory Report ORNL-4628.

Reeves, M.; Cranwell, R.M. (1981) User's manual for the Sandia waste-isolation flow and transport model. Sandia National Laboratories Report NUREG/CR-2324, November.

Papadopulos, S.S.; Larson, S.P. (1978) Aquifer storage of heated water: part II -- numerical simulation of field results. Ground Water 16:242-48.

SOURCE: SWIFT was developed by R. T. Dillon at Sandia Laboratories and by R. B. Lantz and S. B. Pahwa at Intera, Incorporated.

CODE NAME: SWIP2

PHYSICAL PROCESSES: Predicts the effects of liquid waste disposal in deep saline aquifers.

DIMENSIONALITY: Three dimensional (cartesian or radial).

SOLUTION TECHNIQUE: Numerical, finite difference.

DESCRIPTION: SWIP2 is a transient, three-dimensional subsurface waste disposal model to provide methodology to design and test waste disposal systems. The model is a finite-difference solution to the pressure, energy, and mass-transport equations. Equation parameters such as viscosity and density are allowed to be functions of the equations' dependent variables. Multiple user options allow the choice of x, y, and z cartesian or r and z radial coordinates, various finite-difference methods, iterative and direct matrix solution techniques, restart options, and various provisions for output display. Well-bore heat and pressure-loss calculation capabilities are also available.

The 1979 update of the SWIP model involved additions and modifications to include free water surface, vertical recharge, equilibrium controlled linear adsorption, and a first-order irreversible rate reaction. These modifications make this model more adaptable to general hydrologic problems and those involving waste disposal with simple chemical reactions.

CODE INPUT: Unknown.

CODE OUTPUT: Unknown.

COMPILATION REQUIREMENTS: SWIP2 is written in FORTRAN and implemented on a CDC machine.

EXPERIENCE REQUIREMENTS: Extensive.

TIME REQUIREMENTS: Months.

CODE VERIFICATION: Unknown.

DOCUMENTATION/REFERENCES:

INTERA Environmental Consultants, Inc. (1976) A model for calculating effects of liquid waste disposal in deep saline aquifer, part I -- development, part II -- documentation. Houston, TX, June.

INTERA Environmental Consultants, Inc. (1979) Revision of the documentation for a model for calculating effects of liquid waste disposal in deep saline aquifers. U.S. Geological Survey, Water Resources Investigations 79-96.

SOURCE: SWIP2 was developed by INTERA Environmental Consultants, Incorporated. This code is in the public domain.

*U.S. Government Printing Office 1988: 548-158/87005