NUREG/CR-2782

A Summary of Repository Siting Models

Final Report

Prepared by S. D. Thomas, B. Ross, J. W. Mercer

GeoTrans, Inc.

Teknekron Research, Inc.

Prepared for
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Commission

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ABSTRACT

This report is the first in a series of reports that will provide critical reviews and summaries of computer programs that can be used to analyze the potential performance of a high-level radioactive waste repository. The computer programs identified address the following phenomena: saturated and unsaturated subsurface flow, heat transport, solute transport, surface water runoff, geomechanical interactions, and geochemical interactions. The report identifies 183 computer programs that can be used to analyze a repository site and provides a summary description of 31 computer programs. The summary descriptions can be used: to assist in code evaluation, to facilitate code comparison, to determine applicability of codes to specific problems, to identify code deficiencies, and to provide a screening mechanism for code selection.

CONTENTS

CONTENTS (Continued)

LIST OF FIGURES

LIST OF TABLES

PREFACE

We gratefully acknowledge the assistance of Dr. Noel Krothe in the preparation of the summaries for the geochemistry codes. We would also like to acknowledge the assistance of Dr. Mary Anderson and Mr. Joseph Fischer in critically reviewing this manuscript as members of Teknekron's External Quality Assurance Team. The completion of this manuscript in a timely fashion was made possible by the diligent efforts of Ms. Darlene Eamigh, Mrs. Carol Roberts, and Mrs. Phyllis Konikow.

This work was performed under subcontract to Teknekron Research, Inc., whose project manager, Mr. Douglas Vogt, provided valuable assistance. The study was performed for the U.S. Nuclear Regulatory Commission (NRC Contract Number NRC-02-81-026). The NRC project officers were Mr. Stewart Silling and Ms. Linda Lehman. The review was performed by Stephen Thomas, Benjamin Ross, and James Mercer. In addition to his other help on this project, Dr. Ross assisted in summarizing published information on the code NUTRAN; however, the critical review of this code was made by the other authors.

1.0 INTRODUCTION

1.1 PURPOSE OF THIS REPORT

The effective management of high-level radioactive wastes is essential to protect public health and safety. The Department of Energy (DOE), through responsibilities inherited from the Energy Research and Development Administration (ERDA) and the Atomic Energy Commission (AEC), is responsible for the safe disposal of these wastes. The Nuclear Regulatory Commission (NRC), through authority granted it by the Energy Reorganization Act of 1974 that created NRC, is responsible for the regulation of high-level waste management.

The Environmental Protection Agency (EPA) has the authority and responsibility for setting generally applicable standards for radiation in the environment. The NRC is responsible for implementing these standards in its licensing actions and assuring that public health and safety are protected. Although no EPA standards for disposal of high-level radioactive wastes (HLW) yet exist, the NRC has proposed technical criteria for regulating geologic disposal of HLW. These proposed technical criteria have been developed to be compatible with a generally applicable environmental standard. The performance objectives and criteria address the functional elements of geologic disposal of HLW and the analyses required to give confidence that these functional elements will perform as intended. These technical criteria are described in 10 CFR Part 60 (Code of Federal Regulations) and in a draft report containing a list of issues.

In discharging its responsibility, the NRC must review DOE performance assessments and independently evaluate the performance of the repository(ies) that DOE seeks to license. Because of the complexity and multiplicity of these performance assessments, computerized simulation modeling is used. Computer simulation models provide a framework to incorporate the most important processes that will be active in a repository, thereby permitting assessment and prediction of repository behavior. The time frames, ranging from decades to hundreds of millenia, associated with high-level waste management also necessitate the use of models.

To meet this demand, the NRC is developing models and computer codes for supporting these regulations and for performing reviews of proposed nuclear waste management systems. The DOE is also independently developing models and computer codes to assess repository sites and designs. As part of model and code development, a procedure for independent evaluation of the reliability of these models and codes is required. Codes must be evaluated to determine the limitations of theories and the reliability of supporting empirical relations and laboratory tests used for evaluation of long-term repository performance.

The purpose of this report is to provide critical summaries of a variety of codes which are candidates for benchmarking by NRC. The summaries can be used:

- as independent evaluations of the codes
- to facilitate comparison of codes
- to determine which codes are applicable to a given NRC requirement
- as an indication of potential deficiencies of the codes
- to provide a screening mechanism for code selection.

1.2 SCOPE OF THIS REPORT

This report is the first in a series of reports that, as a whole, will provide an independent evaluation of models. The models used for repository performance assessment have been divided into the following categories: (1) repository siting, (2) dosimetry, (3) repository design, (4) waste package performance, and (5) overall systems.

Repository siting codes are codes for analysis of: saturated flow, unsaturated flow, surface water flow (flood routing), solute transport, heat transport, combined solute and heat transport, geochemistry, and geomechanics.

Radiation dosimetry codes include computer programs used to calculate dose-to-man. The dosimetry codes will include computer programs for analyzing: radionuclide source terms, the drinking water pathway, the atmospheric pathway, the immersion pathway, and the food pathway. The dosimetry codes will be used to calculate the concentration of radionuclides in the environment, the resulting dose-to-man, and expected mortality rates.

The repository design codes will be used for analysis of: heat transport, repository handling accidents, flow in fractured media, solute transport, geomechanical analyses, saturated flow, and structural design.

Waste package codes will be capable of performing analyses of the very near-field, primarily those interactions taking place within the waste package to its interactions with repository host rock. The waste package codes will be capable of analyzing chemical interactions such as corrosion, as well as heat transfer and thermal and mechanical stress.

Overall systems codes will analyze one or more of the subcategories of the major code categories. For example, overall systems codes may analyze one or more aspects of: radiation dosimetry, waste package performance, economic cost (e.g., cost/benefit analysis), repository performance, natural multi-barrier performance, or probabilistic aspects of repository performance. Solute transport is a major component of many systems codes, and some of the solute transport codes treated under repository siting are parts of systems codes.

This report considers only repository siting codes. The first step in evaluating the codes is to select codes (the ones summarized in this report) that can be used for repository assessment. The next step is to prepare summaries describing the selected codes and then to prepare benchmark problems for testing them. As a prerequisite to designing benchmark problems, data that will be used in the benchmark problems should be summarized. Thus, three reports will be prepared on repository siting codes: (1) a model summary report, (2) a data set report, and (3) a benchmark problem report. This report is the model summary report for repository siting codes.

The main body of this report summarizes the codes, with each chapter discussing a different type of code. The summaries follow a standard format (shown in Table 1-1) and are based on available publications and documentation, supplemented in some cases by the experience of members of the project team. The summaries are not comprehensive; rather, the goal was to indicate how the codes might be used in siting a waste repository and point out any deficiencies in the codes. Because of the time constraints in preparing this report, only a limited review could be performed, and we do not expect that all flaws in the models have been identified. In many cases it was not possible to evaluate the validity and completeness of the codes. It was also necessary to use mathematical notations which differed among summaries in some cases. These summaries represent an early step in a screening process; a more detailed evaluation will be performed on those codes that are eventually selected for benchmarking.

A number of documents are available which summarize large numbers of radioactive waste management or geohydrology computer codes. A listing of these is given in Appendix A. This report differs from past efforts by presenting more detail and more evaluation on the codes it describes.

1.3 CODE SELECTION METHOD

The codes summarized here were selected as part of a three-step process. The first level in the code selection process was to assemble lists of relevant codes which are available in the literature. The codes reviewed in this step and the lists from which they were drawn are listed in Appendix A.

The next step in model selection was to identify the computer codes that the DOE might use to prepare a license application and the codes that the NRC might use for independent analyses and checks of the DOE calculations. The codes selected in this step are summarized in this report. The selection criteria for this second level of model selection may be summarized as follows:

- Codes currently being used by DOE and NRC should be selected.

Table 1-1

Standard Format for Code Summaries

I. Summary of Code

- Purpose and Scope
- Authors
- Code Functions
- Potential Usage
- Related NRC Issues
- Restrictions

II. Summary of Findings

- General Critique
- Applicability to Medium
- Sensitivity Analysis
- Code Verification
- Field Validation

III. General Characteristics

- Operating Characteristics
- Inputs
- Outputs
- Available Documentation

IV. Review of Theory

- Equations
- Numerical Approximations
- Probabilistic or Statistical Aspects
- Assumptions and Simplifications
- Structure and Level of Detail
- Major Dependent Variables
- Applicability, Limitations, Validity, and Completeness
- References

- Other codes most likely to be of use to NRC should be included as well. These codes should satisfy at least one of the following:
  - performs a function not included in NRC codes
  - may be superior to NRC codes under some circumstances
  - widely used and generally accepted
  - used by USGS.

- These codes should be:
  - unclassified
  - documented sufficiently to make preparation of a summary feasible.

- If codes are available in several versions, the most recent should be used.

- The total number of codes reviewed must be consistent with the project budget.

The third and final level of selection is to determine which of the codes summarized should actually be benchmarked. Recommendations for this selection will be made in a letter report.

1.4 PROCESSES CONSIDERED

Only repository site evaluation is considered in this report. The processes that are important are (1) saturated ground-water flow, (2) unsaturated flow, (3) surface water flow, (4) geochemistry, (5) heat transport, (6) solute transport, and (7) geomechanics. Probably the most important of these processes are saturated ground-water flow and solute transport. Unsaturated flow will be important if a repository is sited above the water table. For repository siting, only "flood-routing" surface water codes are considered. Transport of radionuclides by surface water will be considered under the dosimetry category. Some heat transport codes are considered, but this area will be covered in more detail under the repository design category. For geomechanics, codes dealing with consolidation are generally considered; other geomechanical codes are considered in the repository design category. These qualitative guidelines played a role in determining how many codes were selected under each process.

The codes that are described in this report are divided according to the processes they model. The codes are presented in the following order: (1) saturated flow codes, (2) unsaturated flow codes, (3) surface water flow codes, (4) geochemistry codes, (5) heat transport codes, (6) solute and heat transport codes, (7) solute transport codes without heat transport, and (8) geomechanical codes. Within these sections, some of the codes consider different types of media, such as porous and fractured. Also, some codes can model more than one type of process, as shown in Figure 1-1. These codes are listed under the most complex type of problem they solve.

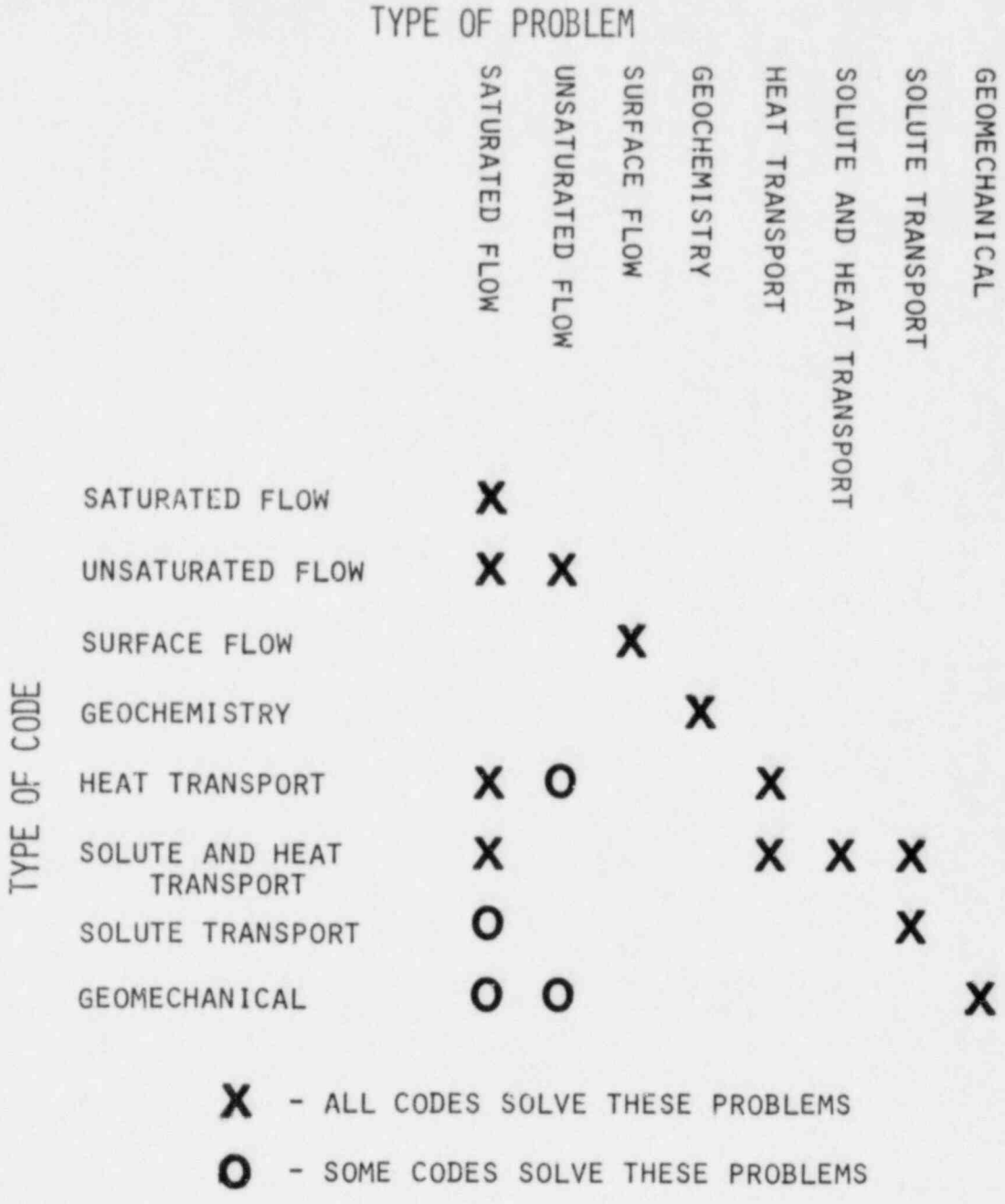

Figure 1-1. Types of Problems Solved by Each Type of Code

The principal features of the codes summarized in this report are shown in Table 1-2. The number of codes of each code type, shown in Table 1-3, indicates in a rough way the relative importance of that type to repository siting. For example, heat transport and geomechanical codes are not considered to be as important to repository siting as saturated flow. The principal exception to this tendency is unsaturated flow. In our review of codes for the various code types, it was observed that an adequate number of codes existed for each of the code types, except for transport in the unsaturated zone. The quality of these codes will be evaluated in the course of future work in this project.

1.5 RELATIONSHIP TO NRC ISSUES

The NRC staff has identified a number of issues which would have to be addressed in reviewing a Site Characterization Report. Resolution of these issues would not necessarily imply that an application satisfies the regulations, but the issues would be an important element of the review process.

In order to facilitate use of this report by NRC staff, we have listed the siting issues which each code might be used to address. The full text of each issue addressed by any of the codes (taken from an unpublished staff document) is listed in Table 1-4. The individual summaries simply list the issues by number. Only issues relevant to siting are listed; repository design and waste package issues which some of the codes can address are omitted.

Table 1-2.

Repository Siting Models

MODEL	SOLUTION PROCEDURE	DIMENSIONS	LANGUAGE	MEDIA	PROCESS MODELED
COOLEY	FE	2	FORTRAN	G	SF
FE3DGW	FE	3	FORTRAN	G	SF
USGS2D	FD	2	FORTRAN	G	SF
USGS3D	FD	3	FORTRAN	G	SF
VTT	FD	2	FORTRAN	G	SF
V3	FD	2	FORTRAN	G	SF
FEMWATER	FE	2	FORTRAN	G	SF,U
UNSAT 2	FE	2	FORTRAN	G	SF,U
HEC-1	Sub-basin	2	FORTRAN	Surface	SWF
MITCAT	Sub-basin	2	FORTRAN	Surface	SWF
PHREEQE	--	-	FORTRAN	-	GC
EQ3/EQ6	--	-	FORTRAN	-	GC
WATEQ	--	-	FORTRAN or PL/I	-	GC
CCC	IFDM	3	FORTRAN	G	SF,HT,GM
SHAFT79	IFDM	3	FORTRAN	G	SF,HT
MAGNUM2D	FE	2	FORTRAN	G,F,DP	SF,HT
SHALT	FE	2	FORTRAN	G	SF,HT,ST,HC
SWIFT	FD	3	FORTRAN	G	SF,HT,ST,HC
CHAINT	FE	2	FORTRAN	F	ST
MMT	PT	2	FLECS	G	ST
NWFT/DVM	PN/PT	2	FORTRAN	G,F	SF,ST

Table 1-2 (Continued)

Repository Siting Models

MODEL	SOLUTION PROCEDURE	DIMENSIONS	LANGUAGE	MEDIA	PROCESS MODELED
GETOUT	A	1	FORTRAN	G,F	ST
DPCT	FE,PT	2	FORTRAN	G	SF,ST
NUTRAN	PN	3	PL/I	G,F	ST
AT123D	A	3	FORTRAN	G	ST
KONBRED	FD,MC	2	FORTRAN	G	SF,ST
FEMWASTE	FE	2	FORTRAN	G	ST
PATHS	A	2	FORTRAN	G	SF,ST
DNET	PN	2	FORTRAN	G,F	SF,DS
TRUST	IFDM	3	FORTRAN	G	SF,U,GM
ROCMAS	FE	2	FORTRAN	G,F	SF,GM

ABBREVIATIONS

A - Analytical Solution
DP - Double Porosity Media
DS - Dissolution
F - Fractured Porous Media
FD - Finite Difference
FE - Finite Element
G - Granular Type Porous Media
GC - Geochemistry
GM - Geomechanical
HC - Coupled Heat and Solute Transport
HT - Heat Transport
IFDM - Integrated Finite Difference Method
MC - Method of Characteristics
PN - Pipe Network
PT - Particle Tracker
SA - Semi-Analytical
SF - Saturated Flow
ST - Solute Transport
SWF - Surface Water Flow
U - Unsaturated Flow

Table 1-3. Summary of Code Types

Code Type	Number of Codes Summarized
Saturated Flow	6
Unsaturated Flow	2
Surface Water Flow	2
Geochemistry	3
Heat Transport	3
Solute and Heat Transport	2
Solute Transport	10
Geomechanical	3
Total	31

Table 1-4. List of NRC Issues Addressed by Siting Codes

ISSUE #3	Has the geologic setting been selected and the subsurface facility designed "so as to assure that releases from the geologic repository following permanent closure conform to such generally applicable environmental radiation protection standards as may have been established by the Environmental Protection Agency?" (60.111 (b)(1))
ISSUE #7	Will the geologic setting mitigate the impacts of premature failure of the engineered system during the containment period? (60.111 (b)(3)(i))
ISSUE #8	Will the geologic setting, in conjunction with the engineered system, be capable of isolating radioactive waste following the containment period so that transport of radionuclides to the accessible environment will be in amounts and concentrations that conform to such generally applicable environmental standards as may have been established by the Environmental Protection Agency? (60.111 (b)(3)(ii))
ISSUE #14	Is the geologic repository "located so that pre-waste emplacement ground-water travel times through the far field to the accessible environment are at least 1,000 years?" (60.112 (c))
ISSUE #17	Does the geologic setting have a "host rock that provides the following ground-water characteristics - (1) low ground-water content; (2) inhibition of ground-water circulation in the host rock; (3) inhibition of ground-water flow between hydrogeologic units or along shafts, drifts, and boreholes; and (4) ground-water travel times, under pre-waste emplacement conditions, between the underground facility and the accessible environment that substantially exceed 1,000 years?" (60.122 (f))
ISSUE #18	Does the geologic setting have "geochemical conditions that (1) promote precipitation or sorption of radionuclides; (2) inhibit the formation of particulates, colloids, and inorganic and organic complexes that increase the mobility of radionuclides; and (3) inhibit the transport of radionuclides by particulates, colloids, and complexes?" (60.122 (g))
ISSUE #22	Does the geologic setting show "potential for failure of existing or planned man-made surface water impoundments that could cause flooding of the geologic repository operations area?"

ISSUE #23 Does the geologic setting show "potential, based on existing geologic and hydrologic conditions, that planned construction of large-scale surface water impoundments may significantly affect the geologic repository through changes in the regional ground-water flow system?" (60.123 (a)(2))

ISSUE #24 Does the geologic setting show "potential for human activity to affect significantly the geologic repository through changes in the hydrogeology?" (60.123 (a)(3))

ISSUE #27 Does the geologic setting have a "potential for adverse impacts on the geologic repository resulting from the occupancy and modification of floodplains?" (60.123 (a)(6))

ISSUE #28 Does the geologic setting have a "potential for natural phenomena such as landslides, subsidence, or volcanic activity of such a magnitude that large-scale surface water impoundments could be created that could affect the performance of the geologic repository through changes in the regional ground-water flow?" (60.123 (a)(7))

ISSUE #35 Does the disturbed zone show a "potential for creating new pathways for radionuclide migration due to presence of a fault or fracture zone irrespective of the age of last movement?" (60.123 (b)(7))

ISSUE #40 Does the disturbed zone show a "potential for changes in hydrologic conditions that would significantly affect the migration of radionuclides to the accessible environment including, but not limited to, changes in hydraulic gradient, average interstitial velocity, storage coefficient, hydraulic conductivity, natural recharge, potentiometric levels, and discharge points?" (60.123 (b)(12))

ISSUE #41 Does the disturbed zone show "conditions in the host rock that are not reducing conditions?" (60.123 (b)(13))

ISSUE #42 Does the disturbed zone show "ground-water conditions in the host rock, including but not limited to, high ionic strength or ranges of Eh-pH, that could affect the solubility and chemical reactivity of the engineered systems?" (60.123 (b)(14))

ISSUE #43 Does the disturbed zone show evidence of "processes that would reduce sorption, result in degradation of the rock strength, or adversely affect the performance of the engineered system?" (60.123 (b)(15))

ISSUE #44 Does the disturbed zone show "rock or ground-water conditions that would require complex engineering measures in the design and construction of the underground facility or in the sealing of boreholes and shafts?" (60.123 (b)(16))

ISSUE #75 Is the underground facility designed to accommodate the anticipated response of the bulk geomechanical, hydrogeologic, and geochemical systems to the maximum design thermal loading, given the pattern of fractures and other discontinuities and the heat transfer properties of the rock mass and ground water? (60.21 (c)(1)(i)(F) and 60.132 (k))

2.0 SATURATED FLOW CODES

2.1 COOLEY

Area: Repository Siting

I. Summary of Code

Purpose and Scope - COOLEY was developed to predict the transient or steady-state hydraulic head distribution and velocity flow field in a confined, semiconfined, or unconfined aquifer.

Authors - COOLEY was developed at the Center for Water Resources Research, Desert Research Institute, University of Nevada by R.L. Cooley.

Code Functions - 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 concept 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.

Potential Usage - A major factor in the movement of radionuclides in a hydrologic system is the transport within the ground-water flow. As an input to a code that analyzes the movement of a contaminant, it is necessary to calculate a velocity field. This velocity field is part of the output from COOLEY.

COOLEY is considered a far-field code in the sense that the flow is analyzed outside the disturbed zone.

Related NRC Issues (see Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - This code is public and is therefore available to the NRC.

II. Summary of Findings

General Critique - This is a particularly well documented code and has been well tested, both analytically and in the field. The code is probably more difficult to use than an equivalent finite-difference code, and it does not offer more accuracy.

Only two saturated flow codes based on the finite-element method are described in this report. This code is restricted to two-dimensional flow conditions, whereas the other finite-element code, FE3DGW, treats three-dimensional flow. COOLEY also contains special treatment for unconfined aquifers. This is probably not of particular value for high-level radioactive waste disposal.

COOLEY is best suited for a single layer aquifer system. Only saturated flow is analyzed, but the aquifer may be confined, unconfined or semiconfined. A layered aquifer system, however, may be analyzed when using the radial coordinate system.

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.

Applicability to Medium - 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.

Sensitivity Analysis - An analysis of the sensitivity of results to the choice among the three solution methods available was made. This was done by running five different examples for each of the solution methods.

Code Verification - The code was run for four problems to which analytical solutions were available.

Field Validation - COOLEY was used to simulate the influence of seasonal pumping of irrigation wells on ground-water levels in Ash Meadows, California and Nevada.

III. General Characteristics

Operating Characteristics - 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 6400 computer. COOLEY is programmed in FORTRAN IV.

Inputs - Inputs for 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
Initial hydraulic head distribution

Outputs - Output for COOLEY consists of the pressure distribution and velocity field at each time step.

Available Documentation - COOLEY is documented in Ref. 1.

IV. Review of Theory

Equations - The continuity equation generally assumed to approximately govern ground-water flow when referred to Cartesian coordinates is

$$-\frac{\partial q_i}{\partial x_i} = S_s \frac{\partial h}{\partial t} - W \qquad (2.1)$$

where q_i is the component of specific discharge in the x_i Cartesian coordinate direction, h is hydraulic head, t is time, S_s is specific storage, W is a source-sink term, positive for a source, and Cartesian tensor notation has been used.

Equation (2.1) is written for a three-dimensional coordinate system, and numerical solutions of it are, in theory, no more difficult than for the two-dimensional version. However, because of difficulties associated with basic data acquisition, computer storage requirements, computer run times, and volume of computer program input, it is advisable to reduce the dimensionality of Equation (2.1) whenever possible. This may be accomplished through the process of integration over an interval in one of the coordinate directions.

To arrive at an equation which is approximately valid for unconfined flow, the upper limit of integration in the z direction, z_u, is replaced by H, that is the water table elevation. This equation may take the form of the Boussinesq equation (ref. 2, p. 378) through use of assumptions analagous to the Dupuit-Forchheimer assumptions (ref. 2, pp. 361-366) and the assumption (ref. 1, p. 8) is given as

$$\frac{\partial}{\partial x_i}\left[K_{ij}\,(\bar{h} - z_L)\,\frac{\partial \bar{h}}{\partial x_j}\right] + \frac{q_{Ln}}{n_{L3}} = \left[S_y + S_s\,(\bar{h} - z_L)\right]\frac{\partial \bar{h}}{\partial t} - I - V_s \qquad (2.2)$$

where K_{ij} is the hydraulic conductivity tensor, S_y is the specific yield, $\bar{h}$ the head value averaged over the z direction, z_L the elevation of the aquifer bottom, I the infiltration rate, and V_s the total of source-sink terms in the z direction.

The term q_{Ln}/n_{L3} may represent known recharge or discharge such as, for example, evapotranspiration. It may also be used to approximate leakage into or out of the interval between z_L and z_u. For areal flow analysis involving an aquifer sandwiched between two aquitards, the permeability contrast between the aquifer and each of the aquitards is often great enough that nearly vertical flow can be assumed in the aquitards.

Numerical Approximations - The principal numerical approximations in COOLEY are the following:

- Discretization of space by the finite-element method by 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.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The main assumptions are:

- 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.
- 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.

Structure and Level of Detail - 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.

Major Dependent Variables - The major variables, other than the inputs, are the heads and water velocities.

Applicability, Limitations, Validity and Completeness - COOLEY is most applicable to either an aquifer system in which the flow is predominantly horizontal or a system in which the flow is predominantly radial.

The code would be inapplicable (1) if the flow is strongly three dimensional; an appropriate three-dimensional model must then be used, (2) if the Dupuit-Forchheimer assumptions are not valid, and (3) if gradients of temperature or salinity affect the velocity distribution.

Some versions of COOLEY only model confined flow. The user's manual describes how one would modify them in order to incorporate unconfined flow. It would be advantageous to obtain a version with this modification already implemented.

References -

1. Cooley, R.L., "Finite element solutions for the equations of groundwater flow," Nevada University, January 1974.

2. Bear, J., Dynamics of Fluids in Porous Media, American Elsevier, New York, 1972.

3. Zienkiewicz, O.C., The Finite Element Method in Engineering Science, McGraw-Hill, London, 1971.

2.2 FE3DGW Area: Repository Siting

I. Summary of Code

Purpose and Scope - FE3DGW is a hydrologic model that defines the ground-water flow field and provides water flow paths and travel times. It is a three-dimensional, finite-element code for simulating saturated ground-water flow in a homogeneous or heterogeneous geological system.

Authors - Written by S.K. Gupta, C.R. Cole and F.W. Bond, FE3DGW was 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 Functions - This model is capable of simulating single-layered systems having variable thickness or multilayered systems, where not only thickness can be varied, but the number of layers can be changed to agree with the vertical geological section. Variable spacing may be used and source or sink terms can be defined at a given point (well) or along a given line (rivers, streams, etc.) or for a given region (variable surface infiltration from natural precipitation or irrigation). Pumping stresses in each layer of the subregion can be defined as a function of time. The geologic input data for such complex multilayered systems are reduced to well-log descriptions at each surface node and subdivision of the entire region into two-dimensional elements. Auxiliary programs have been developed to plot grid values, contour maps, and three-dimensional charts of both the input data used in simulation and the results obtained.

Potential Usage - Some of the complex generic and site-specific geologic configurations consist of multi-aquifer systems separated by confining beds. Two aquifers connected by a leaky bed will both respond to stresses imposed on either aquifer. Such coupling of aquifers requires modeling all of the layers simultaneously. A three-dimensional model provides a realistic means of representing multilayered aquifers associated with generic or specific repository sites.

FE3DGW is considered a far-field code in the sense that the flow is analyzed outside the disturbed zone.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - This program is public and therefore is available to the NRC.

II. Summary of Findings

General Critique - The principal advantages of FE3DGW is its ability to simulate three-dimensional systems. A one- or two-dimensional finite-element code should be used for problems which can be solved in fewer dimensions.

FE3DGW has been designed specifically to run on a computer with small-core storage capabilities (minimum of 32 k). However, the penalty for this is the additional computer time required due to the storage of intermediate results on disk, which are repeatedly read and written to minimize the storage required in core.

It is important that care be taken when implementing a fully three-dimensional model. For example, when modeling a layered aquifer system of high and low permeabilities, the low-permeability layer would need to be represented by a number of discretized layers; this is very inefficient. A better representation would be a pseudo 3-D code such as USGS3D in which the leakage from the aquitards may be represented by semianalytic or analytic solutions.

A three-dimensional code is mainly of use for the case when three-dimensional flow is dominant. However, due to the complexity and time required in the input data preparation and the amount of storage and cpu time required, a fully 3-D model should be used only when absolutely necessary. 3-D finite-element codes (unlike finite-difference codes) are very inefficient when used for problems of lower dimensionality.

The code has been extensively used by primarily one group, PNL. The reason for this is the machine-dependance of the code. The results, however, have been extensively published and are generally accepted by the research community.

Applicability to Medium - The model is applicable to most porous media, provided that enough data are available to warrant a three-dimensional model. If, for example, modeling is required for a homogeneous, uniform thickness, horizontal aquifer, then it would be more advantageous to use a two-dimensional model with vertical averaging of the velocity and pressure values, as this would greatly reduce the computer storage and time required.

Fractured media can be modeled if they have enough fractures to be represented approximately as porous media.

Sensitivity Analysis - Sensitivity analysis of grid density was conducted using combinations of square and radial elements. With the major source being circular, radial elements were selected near the source and square elements in the remaining portion of the region.

Code Verification - Sensitivity and verification analysis of the three-dimensional model was also accomplished using two-dimensional or quasi-three-dimensional analytic 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).

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

The model has also been applied to the ground-water 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.

III. General Description

Operating Characteristics - Written in FORTRAN IV, the program listing at our disposal is for a PDP-11/45 with requirements for storage of 32 k for 16 bit words. The program is organized to most efficiently reduce the memory requirements on a minicomputer. For a 3D program this is one of the prime factors when considering the core storage requirements.

Reduction of core storage is achieved by using a sequential disk file to store data. The input data for the finite-element simulation are grouped into two major categories, namely, (1) data used at random - nodal coordinates, boundary conditions, etc. and (2) data used in sequential form - element related information. The former is kept in core as it needs to be retrieved constantly. However, as the element related information is required sequentially, element by element, this is handled through disks.

The code is being converted to a CDC mainframe computer. However, the conversion does not involve reoptimizing the program design.

Inputs - Inputs for FE3DGW include:

- Initial heads
- Boundary conditions
- Specific storage
- Hydraulic conductivity in the three Cartesian coordinate directions
- Recharge and discharge rates
- Aquifer geometry

The grid geometry includes node coordinates and node connections, which makes data input for finite-element codes generally more difficult than that for finite-difference codes.

Outputs - The output consists of the heads and velocity vectors at a node at a particular depth and is given after every time step. Supportive programs have been developed to help verify data correctness by plotting the node location, finite element discretization, well log (geologic section) at each node, thickness, top and bottom elevation of each hydrogeologic unit, and boundary conditions specified in the input data file prepared for simulation.

Available Documentation - The theory and documentation are presented in comprehensive form in Ref. 1.

IV. Review of Theory

Equations - Three-dimensional, nonsteady flow is defined by the following equations:(ref. 3)

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) - W = S_s \frac{\partial h}{\partial t} \qquad (2.3)$$

S_s = Specific Storage, L^{-1}

$= \rho g\,(\alpha_p + \phi\beta_p)$

g = gravity field strength, $L\ t^{-2}$

h = head above common datum, L

$$= z + \frac{1}{g}\int_{p_0}^{p} \frac{dp}{\rho(p)} \qquad (2.3a)$$

K_x, K_y, K_z = represents hydraulic conductivity of the saturated flow in the x, y, and z directions, $L\ t^{-1}$

p = fluid pressure, $M\ L^{-1}\ t^{-2}$

W = strength of sink function, t^{-1}

$$= \sum_{i=1}^{n} Q_w(x_i,y_i,z_i,t)\ \delta\ (x-x_i)\delta(y-y_i)\delta(z-z_i) \qquad (2.3b)$$

Q_w = the well discharge from the aquifer, $L^3\ t^{-1}$

δ = Dirac delta function

t = time, t

z = elevation above given datum, L

ϕ = porosity of medium, dimensionless

α_p = compressibility of medium, $Lt^2\ M^{-1}$

β_p = compressibility of liquid, $Lt^2\ M^{-1}$

ρ = density of fluid, $M\ L^{-3}$

i = well index

n = number of wells

Equation (2.3) is for a fixed coordinate system. Compressibility of medium and liquid is considered only in coefficient S_s, called "specific storage" by Hantush(ref. 4) and defined as the "volume of water a unit volume of aquifer releases from storage under a unit decline of head."

Equation (2.3) can be rewritten in a more compact form by defining the operator L as:

$$L(h) \equiv \frac{\partial}{\partial x_\alpha}\left(K_{\alpha\beta}\frac{\partial h}{\partial x_\beta}\right) - Q - S_s\frac{\partial h}{\partial t} = 0 \qquad (2.4)$$

$$\alpha, \beta = 1, 2, 3$$

In the above equation, subscripts α and β are used to describe the three-dimensional flow equation in condensed form.

Numerical Approximations - Equation (2.4) is solved by the Galerkin method. For finite differencing in time, the Crank-Nicolson or central-difference scheme can be used after the first initial step. In past versions of the model, backward difference was used for the initial time step, but in the present model, the computer program has been modified to simulate changes during the time step.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions are as follows:

- 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.

Structure and Level of Detail - The flow field is represented as a three-dimensional grid. Three-dimensional isoparametric elements are used that can be deformed in any of the three coordinate directions. The spatial basis functions for the isoparametric shapes along any element edge may be either linear, quadratic, or cubic in functional form.

Major Dependent Variables - The major variables, other than the inputs, are the heads and fluid velocities.

Applicability, Limitations, Validity and Completeness - Due to the three-dimensional spatial representation, FE3DGW is applicable to most saturated media providing that enough data are available to warrant such a model.

References -

1. Gupta, S.K., C.R. Cole and F.W. Bond, "Finite Element Three Dimensional Ground Water (FE3DGW) Flow Model Formulation, Program Listings and User's Manual," Pacific Northwest Laboratory Report PNL-2939, 1979.

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3. Jacob, C.E., Chapter 5, in Engineering Hydraulics, ed. H. Rouse, pp. 321-386, John Wiley and Sons, New York, 1950.

4. Hantush, M.S., "Modification of theory of leaky aquifers," J. Geophys. Res., Vol. 65, pp. 3713-3725, 1960.

5. Nelson, R.W. and J.A. Schur, "PATHS groundwater hydrogeological model," Pacific Northwest Laboratory Report PNL-3162, 1980.

6. Gupta, S.K., and G.F. Pinder, "Three-dimensional finite element model for multilayered ground-water reservoir of Long-Island, New York," Dept. of Civil Engineering, Princeton University, Princeton, 1978.

7. Gupta, S.K., and K.K. Tanji, "A three-dimensional Galerkin finite element solution of flow through multiaquifers in Sutter Basin, California," Water Resour. Res., Vol. 12, No. 2, pp.155-162, 1976.

2.3 USGS2D Area: Repository Siting

I. Summary of Code

Purpose and Scope - This finite-difference code was developed to simulate ground-water flow in an artesian aquifer, a water-table aquifer, or a combined artesian and water-table aquifer.

Authors - USGS2D was developed at the United States 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.

Code Functions - 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) ground-water flow conditions, (2) source terms, (3) numerical solution techniques, and (4) input-output. The options for ground-water flow conditions include:

- Artesian conditions
- Water-table conditions
- Combined artesian/water-table conditions

Variations of source terms include:

- Transient leakage from confining beds
- Steady leakage from confining beds
- Recharge
- Pumping wells
- Evapotranspiration

Potential Usage - This code was designed to simulate a variety of ground-water flow conditions within an aquifer in which the flow field may be treated using an areal approximation. USGS2D may be used to examine conditions in the regional area.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - USGS2D is available to the public, with both documentation and program easily obtainable. In addition, the U.S. Geological Survey offers some support for certain users and applications.

II. Summary of Findings

General Critique - Of the various ground-water flow models, USGS2D is one of the most widely used. The code is well documented, has been fully debugged, and has been field verified. The code is maintained by the U.S. Geological Survey.

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.

Although the program has many options, it is restricted to two-dimensional, ground-water flow. Therefore, it may have somewhat limited applicability to problems associated with high-level radioactive waste disposal.

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.

Applicability to Medium - USGS2D is designed for most types of geological media where two-dimensional flow in a porous medium can be assumed.

Sensitivity Analysis - Numerous sensitivity calculations have been performed with this code. These sensitivity calculations include both numerical and physical parameters for specific problems. The numerical parameters include (1) matrix solution technique, (2) matrix parameters such as overrelaxation parameters, (3) grid spacing, and (4) time steps. Physical parameters that have been varied include (1) hydraulic conductivity, (2) storage properties, (3) leakage properties, and (4) recharge properties.

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.

Field Validation - This code has been the work horse of the U.S. Geological Survey for about the last 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).

III. General Description

Operating Characteristics - 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.

Inputs - USGS2D may read single or multiple data sets. The contents of a data set are described in Table 2-1.

Table 2-1 Summary of Major Data Requirements for Various Flow-Condition Options and Source Terms in USGS2D

FLOW CONDITIONS	SOURCE CONDITIONS			
	Aquifer Parameters	Leakage	Recharge	Evapotranspiration
Artesian	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	
Water-Table	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 Artesian and Water-Table	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

Outputs - 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.

Available Documentation - Documentation (Refs. 1 and 2) for USGS2D is available in two government publications. The computer card deck can be obtained, at cost, by requesting it from:

Ralph N. Eicher
Chief, Office of Teleprocessing
Mail Stop 805, National Center
U.S. Geological Survey
Reston, Virginia 22092

IV. Review of Theory

Equations - The partial differential equation of ground-water flow in a confined aquifer in two dimensions, where it is assumed that the Cartesian coordinate axes are aligned with the principal components of the transmissivity tensor, may be written as:

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) = S\frac{\partial h}{\partial t} + W(x,y,t) \qquad (2.20)$$

where

T_{xx}, T_{yy} are the principal components of the transmissivity tensor (L^2t^{-1});
h is hydraulic head (L);
S is the storage coefficient (dimensionless);
W is the volumetric flux of recharge or withdrawal per unit surface area of the aquifer (Lt^{-1}).

In water-table aquifers, transmissivity is a function of head. Assuming that the coordinate axes are co-linear with the principal components of the hydraulic conductivity tensor, the flow equation may be expressed as

$$\frac{\partial}{\partial x}\left(K_{xx}\,b\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_{yy}\,b\frac{\partial h}{\partial y}\right) = S_y\frac{\partial h}{\partial t} + W(x,y,t) \qquad (2.21)$$

in which

K_{xx}, K_{yy} are the principal components of the hydraulic conductivity tensor (Lt^{-1});
S_y is the specific yield of the aquifer (dimensionless);
b is the saturated thickness of the aquifer (L).

Numerical Approximations - Equations (2.20) and (2.21) are approximated using a central-difference approximation for the second derivatives in space and a backward-difference approximation for the first derivative in time. Utilizing a block-centered, finite-difference grid in which variable grid spacing is allowed, Equation (2.20) may be

approximated as

$$F_{i,j}(h_{i,j+1,k}-h_{i,j,k})-D_{i,j}(h_{i,j,k}-h_{i,j-1,k})$$
$$+H_{i,j}(h_{i+1,j,k}-h_{i,j,k})-B_{i,j}(h_{i,j,k}-h_{i-1,j,k})$$
$$= \frac{S_{i,j}}{\Delta t}(h_{i,j,k}-h_{i,j,k-1})+W_{i,j,k} \qquad (2.22)$$

in which

$$B_{i,j}=\frac{\left[\dfrac{2T_{yy\,(i,j)}\,T_{yy\,(i-1,j)}}{T_{yy\,(i,j)}\Delta y_{i-1}+T_{yy\,(i-1,j)}\,\Delta y_i}\right]}{\Delta y_i} \qquad (2.23)$$

$$D_{i,j}=\frac{\left[\dfrac{2T_{xx(i,j)}\,T_{xx\,(i,j-1)}}{T_{xx(i,j)}\Delta x_{j-1}+T_{xx(i,j-1)}\Delta x_j}\right]}{\Delta x_j} \qquad (2.24)$$

$$F_{i,j}=\frac{\left[\dfrac{2T_{xx(i,j)}\,T_{xx\,(i,j+1)}}{T_{xx(i,j)}\Delta x_{j+1}+T_{xx\,(i,j+1)}\Delta x_j}\right]}{\Delta x_j} \qquad (2.25)$$

$$H_{i,j}=\frac{\left[\dfrac{2T_{yy(i+1,j)}\,T_{yy\,(i,j)}}{T_{yy(i,j)}\Delta y_{i+1}+T_{yy(i+1,j)}\Delta y_i}\right]}{\Delta y_i} \qquad (2.26)$$

where

Δx_j is the space increment in the x direction for column j (L);
Δy_i is in the space increment in the y direction for row i (L);
Δt is the time increment (t);
i is the index in the y dimension;
j is the index in the x dimension;
k is the time index.

Equations (2.23)-(2.26) represent the harmonic mean for the transmissivity between grid blocks. Equation (2.22) is also used to approximate Equation (2.21) by replacing S with S_y and defining the transmissivities in Equations (2.23)-(2.26) as a function of head. Details on how the source terms are treated are given in the documentation and are not repeated here.

This approximation results in a matrix equation that can be solved by several different methods. The options that are provided by USGS2D are (1) strongly implicit procedure, (2) line successive overrelaxation, (3) alternating direction implicit, or (4) a direct solution using D4 ordering. The last of these options is not included in some versions of the code; it is described in Ref. 2.

Probabilistic or Statistical Aspects - The program contains none.

Assumptions and Simplifications - The major assumptions are as follows:

- 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.

Structure and Level of Detail - 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 code considers several different flow conditions, source term options, and solution techniques.

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

Applicability, Limitations, Validity, and Completeness - The program is limited to two-dimensional (areal) ground-water flow problems. Problems with vertical flows are not handled. Given this limitation, this program can treat most anticipated conditions if such an application is needed.

References -

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2. Larson, S.P., "Direct solution algorithm for the two-dimensional ground-water flow model," U.S. Geological Survey, Open File Report 79-202, 1979.

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2.4 USGS3D — Area: Repository Siting

I. Summary of Code

Purpose and Scope - This finite-difference code was developed to simulate ground-water flow in three dimensions. The code can be used in a fully three-dimensional mode or a quasi three-dimensional mode.

Authors - USGS3D was developed at the United States Geological Survey and is described in a series of open-file reports by P.C. Trescott and S.P. Larson.

Code Functions - 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. If 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.

Potential Usage - This code was designed to simulate a three-dimensional ground-water flow system. It may be used to examine conditions in the regional area.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - USGS3D is available to the public, with both documentation and program easily obtainable. In addition, the U.S. Geological Survey offers some support for certain users and applications.

II. Summary of Findings

General Critique - USGS3D has been used successfully by the U.S. Geological Survey for several field applications including a regional model of the Columbia Plateau (currently in the review process). The program is useful in aiding the understanding of regional flow systems in which high-level radioactive repositories are placed. USGS3D is the only three-dimensional finite-difference saturated flow model discussed in this section. (SWIFT, discussed in Section 7, includes this feature.). As such, it can be used to help address the same issues as FE3DGW. The advantage of USGS3D over FE3DGW is that it is less machine dependent and data input is somewhat easier. On the other hand, FE3DGW is likely to be used by DOE contractors.

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.

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) ground-water 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-time simulations, which approach a steady state, this type of leakage is adequate.

Applicability to Medium - USGS3D is ideally suited for layered systems of aquifers and confining beds, where flow in a porous medium can be assumed.

Sensitivity Analysis - Some sensitivity analyses have been performed on USGS3D. The type of analysis is similar to that performed on USGS2D; however, USGS3D has been used significantly less than USGS2D. Therefore, the sensitivity analysis is also less extensive.

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.

Field Validation - 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.

III. General Description

Operating Characteristics - 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 a 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.

Inputs - 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
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.

Outputs - 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.

Documentation - Documentation (ref. 1 and 2) for USGS3D is available in two U.S. Geological Survey open-file reports. The computer card deck can be obtained, at cost, by requesting it from:

Ralph N. Eicher
Chief, Office of Teleprocessing
Mail Stop 805, National Center
U.S. Geological Survey
Reston, VA 22092

IV. Review of Theory

Equations - The partial differential equation of ground-water flow in three dimensions, where it is assumed that the coordinate axes are aligned with the principal directions of the hydraulic-conductivity tensor, may be written as,

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)=S_s\frac{\partial h}{\partial t}+W(x,y,z,t) \quad (2.27)$$

in which

h is hydraulic head (L);
S_s is specific storage (L^{-1});
K_{xx}, K_{yy}, K_{zz} are the principal components of the hydraulic-conductivity tensor (Lt^{-1});
$W(x,y,z,t)$ is a volumetric flux per unit volume (t^{-1}).

In the finite-difference simulator, it is convenient to represent a hydraulic unit by one layer of nodes. For this approach, Equation (2.27) is multiplied by b, the thickness of the hydrogeologic unit giving approximately

$$\frac{\partial}{\partial x}\left(T_{xx}\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_{yy}\frac{\partial h}{\partial y}\right) + b\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) = S'\frac{\partial h}{\partial t} + bW(x,y,z,t) \quad (2.28)$$

in which T_{xx}, T_{yy} are the principal components of the transmissivity tensor ($L\ t$);
S' is the storage coefficient (dimensionless).

Although the model is designed to solve Equation (2.28), it will solve Equation (2.27) by substituting hydraulic conductivity, specific storage, and $W(x,y,z,t)$ for transmissivity, storage coefficient, and $bW(x,y,z,t)$, respectively.

Numerical Approximations - In order to solve Equation (2.27) or (2.28) for a heterogeneous, anisotropic porous medium with irregular boundaries, the approach taken is to subdivide the region into blocks in which the medium properties are assumed to be uniform. The continuous derivatives in Equation (2.27) or (2.28) are replaced by finite-difference approximations for the derivatives at a point (the node at the center of the block). The result is N equations in N unknowns (head values at the nodes) where N is the number of blocks representing the porous medium.

Utilizing a block-centered, finite-difference grid in which variable grid spacing is permitted, Equation (2.28) may be approximated as

$$\begin{aligned} &F_{i,j,k}\,(h_{i,j+1,k} - h_{i,j,k}) - D_{i,j,k}(h_{i,j,k} - h_{i,j-1,k}) + \\ &H_{i,j,k}\,(h_{i+1,j,k} - h_{i,j,k}) - B_{i,j,k}(h_{i,j,k} - h_{i-1,j,k}) + \\ &S_{i,j,k}\,(h_{i,j,k+1} - h_{i,j,k}) - Z_{i,j,k}(h_{i,j,k} - h_{i,j,k-1}) \\ &= \frac{S'_{i,j,k}}{\Delta t}(h_{i,j,k} - \hat{h}_{i,j,k}) + bW_{i,j,k} \end{aligned} \quad (2.29)$$

in which the carat refers to the previous time step and

$$B_{i,j,k} = \left[\frac{2T_{yy[i,j,k]}T_{yy[i-1,j,k]}}{T_{yy[i,j,k]}\Delta y_{i-1} + T_{yy[i-1,j,k]}\Delta y_i}\right] /\Delta y_i \qquad (2.30)$$

$$D_{i,j,k} = \left[\frac{2T_{xx[i,j,k]}T_{xx[i,j-1,k]}}{T_{xx[i,j,k]}\Delta x_{j-1} + T_{xx[i,j-1,k]}\Delta x_j}\right] /\Delta x_j; \qquad (2.31)$$

$$F_{i,j,k} = \left[\frac{2T_{xx[i,j,k]}T_{xx[i,j+1,k]}}{T_{xx[i,j,k]}\Delta x_{j+1} + T_{xx[i,j+1,k]}\Delta x_j}\right] /\Delta x_j; \qquad (2.32)$$

$$H_{i,j,k} = \left[\frac{2T_{yy[i+1,j,k]}T_{yy[i,j,k]}}{T_{yy[i,j,k]}\Delta y_{i+1} + T_{yy[i+1,j,k]}\Delta y_i}\right] /\Delta y_i; \qquad (2.33)$$

$$S_{i,j,k} = \left[\frac{2(K_{zz})_{i,j,k+1}(K_{zz})_{i,j,k}}{(K_{zz})_{i,j,k}\Delta z_{k+1} + (K_{zz})_{i,j,k+1}\Delta z_k}\right] /\Delta z_k; \qquad (2.34)$$

$$Z_{i,j,k} = \left[\frac{2(K_{zz})_{i,j,k-1}(K_{zz})_{i,j,k}}{(K_{zz})_{i,j,k}\Delta z_{k-1} + (K_{zz})_{i,j,k-1}\Delta z_k}\right] /\Delta z_k. \qquad (2.35)$$

where the bracketed terms of Equations (2.30)-(2.35) represent the harmonic means of the interblock transmissivity or hydraulic conductivity terms and where

x_j is the space increment in the x direction for column j (L);
y_i is the space increment in the y direction for row i (L);
z_k is the space increment in the z direction for layer k (L);
t is the time increment (t);
i is the index in the y dimension;
j is the index in the x dimension;
k is the index in the z dimension.

If the upper unit is under water-table conditions, specific yield is used in place of the storage coefficient and the transmissivity is defined as a function of head for the previous iteration. The iterative matrix technique used to solve the set of simultaneous finite-difference equations is the strongly implicit procedure (SIP).

Probabilistic or Statistical Aspects - The program contains none.

Assumptions and Simplifications - The major assumptions are as follows:

- 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.

Structure and Level of Detail - 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.

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

Applicability, Limitations, Validity, and Completeness - This code is applicable to three-dimensional flow systems surrounding a high-level radioactive waste repository. As noted, this code is being used by the U.S. Geological Survey to examine the regional flow system in the Columbia Plateau. The code is limited to flow only, but the three-dimensional treatment of flow is fairly complete. Results from this code are generally accepted as being valid and correct, when the code is properly applied.

The principal limitation of the code is the difficulty of obtaining enough data to describe a three-dimensional flow system.

References -

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

2. Trescott, P.C. and S.P. Larson, Supplement to open-file report 75-438, "Documentation of finite-difference model for simulation of three-dimensional ground-water flow," U.S. Geological Survey Open-File Report 76-591, 1976.

3. Weeks, J.B., G.H. Leavesley, F.A. Welder, and G.J. Saulneir, Jr., "Simulated effects of oil-shale development on the hydrology of Piceance basin, Colorado," U.S. Geol. Survey Prof. Paper 908, 1974.

2.5 VTT Area: Repository Siting

I. Summary of Code

Purpose and Scope - VTT or Variable Thickness Transient Model is a hydrologic model to define the ground-water flow field and provide water flow paths and travel times.

Authors - Written by A.E. Reisenauer, VTT was a result of research conducted by Pacific Northwest Laboratory and supported by the Waste Isolation Safety Assessment Program (WISAP).

Code Functions - This 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.

Potential Usage - 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.

VTT is considered a far-field code in the sense that the flow is analyzed outside the disturbed zone.

Related NRC Issues (Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - The code is in the public domain and therefore is available to the NRC.

II. Summary of Findings

General Critique - As a quasi-three-dimensional code, VTT is similar to some aspects of USGS3D. The water in an aquifer tends to flow in a horizontal direction along the bedding plane of the more permeable geologic formation since the resistance to flow is less. VTT takes advantage of this horizontal nature of the flow field by transforming the three-dimensional flow equations to a series of coupled two-dimensional problems. If there is a three-dimensional flow field within an aquifer, then it would appear that VTT would not be applicable and a fully three-dimensional model such as FE3DGW or the fully three-dimensional mode of USGS3D would be required.

A significant disadvantage is the fact that formulation of the flow equations and the discretization of the aquifer domain is valid only for uniform grid spacing. This is very restrictive when it is necessary to efficiently model a real aquifer system.

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 model has been validated with other numerical models and analytic solutions; however, it has not, to our knowledge, been validated in the field.

Applicability to Medium - VTT is designed for a layered system. This could be either a sedimentary sequence or an igneous sequence such as layered basalt.

Sensitivity Analysis - None.

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.

Field Validation - None.

III. General Description

Operating Characteristics - Written in FORTRAN IV-PLUS, the program listing is for use on a PDP-11/45. This code is currently being converted to a CDC machine by Intera, Inc.

Inputs - The ground-water model requires the following in order to be run:

Total stress or recharge at each node
Aquifer top elevation
Aquifer bottom elevation
Initial aquifer potential
Aquifer storage coefficient
Interaquifer transfer (leakage) coefficient
Aquifer hydraulic conductivity (or transmissivity) at each node

Perhaps the most difficult of these to obtain are the interaquifer transfer coefficients.

Outputs - The solution 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:

- ground-water velocities
- ground-water flowpaths

- travel times
- 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.

Available Documentation - The theory and documentation (Ref. 1) is presented in comprehensive form.

IV. Review of Theory

Equations - Often an exact solution of the general, three-dimensional, saturated flow equation and free-surface boundary condition is not required to obtain useful results. VTT utilizes the Dupuit-Forchheimer or Boussinesq approximate method, which assumes a simplified, two-dimensional horizontal view of the ground-water system. This allows the free-surface boundary condition and the flow equation to be combined into a single equation amenable to practical numerical solution techniques. For simplicity we will refer to this method as the Boussinesq flow model.

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

$$q_x = \phi \frac{dx}{dt} \tag{2.36}$$

$$q_y = \phi \frac{dy}{dt} \tag{2.37}$$

$$q_z = \phi \frac{dz}{dt} \tag{2.38}$$

where:

ϕ = effective porosity.

With the coordinate of the free surface represented by $z = h(x, y, t)$, the Dupuit assumptions used in this model may be simply stated as: $\psi(x, y, z, t) \simeq \psi(x, y, \overline{z}, t)$, where $\overline{z}$ = average height of the water particles above reference datum. This is equivalent to stating that flow is essentially horizontal, so that vertical flow components can be neglected and that the slope of the water-table surface is slight (<5°). If it is assumed that the fluid is incompressible and the flow system is fully saturated, then the equation of continuity written in terms of Darcian velocities becomes:

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = 0 \qquad (2.39)$$

In order to average flow in the z-direction, this equation must be integrated from the base of the aquifer to the free surface.

Additionally, it may be shown that with Darcy's law rewritten as:

$$q_x = -\overline{K} \frac{\partial h}{\partial x}$$
$$q_y = -\overline{K} \frac{\partial h}{\partial y} \qquad (2.40)$$

where $\overline{K}(x, y)$ is the vertically averaged value of hydraulic conductivity at location (x, y), the governing equation describing the flow of incompressible fluid in an unconfined aquifer, known as the Boussinesq equation, is given as:

$$\Phi \frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left(\frac{\overline{K}h\partial h}{\partial x}\right) - \frac{\partial}{\partial y}\left(\frac{\overline{K}h\partial h}{\partial y}\right) = 0 \qquad (2.41)$$

Furthermore, the equation required to handle an aquifer with varying bottom elevation $h^b(x, y)$ and to include source/sink or accretion terms is given as:

$$\overline{\Phi} \frac{\partial h}{\partial t} = \nabla \cdot \overline{K} (h-h^b) \nabla h + N \qquad (2.42)$$

where:

$\overline{\Phi}(x, y)$ = vertical average of the effective porosity of the aquifer (dimensionless)

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

$h^b(x, y)$ = elevation of the aquifer bottom from the reference elevation (L)

$N(x, y)$ = accretion rate (Lt^{-1})

$K(x, y)$ = vertically averaged value for hydraulic conductivity at point (x, y) (Lt^{-1})

Equation (2.42) is valid assuming that, as in the case for the free surface, the bottom slope is slight.

The Boussinesq flow model requires initial conditions. The Boussinesq flow model requires one average potential value for each aquifer for each (x, y) grid location throughout the region being modeled.

Solving the flow equation requires that boundary conditions be specified. Boundary conditions are difficult to formulate and result from interpretations of potential data, well logs, and lithologic data. The physical extent of the aquifer and or aquifers are defined. This includes a geometrical description of the positions in space of the aquifer materials such as:

- the lateral boundaries of the aquifer or aquifer systems.
- contour maps of the base and top of the aquifer or aquifer systems.

Along each of the lateral boundaries, the conditions which describe the physical situation must be determined. These include:

- Lateral flow boundaries that result from not extending the model to the geologic boundaries of the aquifer or aquifer systems. At these boundaries the rate that water is flowing into or out of the aquifer or aquifer system must be specified.
- No-flow boundaries which occur when the model has been extended to the geologic boundaries of the aquifer where the aquifer materials and impermeable barriers meet.
- Constant or time-varying potential boundaries that occur at large lakes and rivers, where the saturated aquifer materials are in contact with large bodies of water whose water-surface elevations are essentially unaffected by aquifer potentials.

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

Three different solution techniques are selected to solve essentially the same set of equations, thus resulting in three separate versions of the same model. Each of these is designed for use in specific problems.

The VTT version of the model solves the transient form of the system of finite-difference equations by using the line successive overrelaxation technique. For transient problems the solution is stable and convergent with sufficient speed to make solution of large matrices practical.

The VTTSS3 version of the model solves the steady-state system of finite-difference equations resulting from Equation (2.42) when the transient term is set to zero. This set of equations is solved by using a Newton iteration technique. This version is primarily used for a system of aquifers in which one is unconfined and, therefore, the equations are nonlinear. Convergence of this method is quadratic in nature and for most ground-water problems the solution is reached in four to five iterations.

The VTTSSZ version of the model solves the same system of steady-state equations discussed in the preceding paragraph, except that it uses a Cholesky decomposition method (ref. 3). This version is used when all the aquifers being simulated are confined. This method is many times faster than the Newton version, and since the system of equations will be linear, no iteration is required.

Some other numerical approximations are:

- Coefficient distributions and dependent variables are assumed continuous over the simulation region.

- Impermeable boundaries must be straight or have a 135° angle at any node.

Probabilistic or Statistical Aspects - None.

Assumptions or Simplifications - The basic assumptions of the Boussinesq flow model for describing saturated unconfined flow 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 inhomogeneous.

- The free-surface slope and the aquifer bottom slope are both slight ($<5°$).

- Vertical velocities are small and can be neglected.

- Flow in the capillary fringe is neglected.

- Seepage surfaces cannot be handled and are neglected.

Structure and Level of Detail - The flow field is represented as a sequence of aquifers. Each aquifer is modeled as a grid of identical rectangular cells.

Major Dependent Variables - The major variables, other than the inputs, are the head and water velocities.

Applicability, Limitations, Validity, and Completeness - This code is applicable to flow systems surrounding a high-level radioactive waste repository. The code VTT has been used by the staff at Pacific Northwest Laboratories (PNL) to simulate the regional system at the Columbia Plateau. The regional model covered 21,000 square miles and had two active layers, which were connected through the use of transfer coefficients. It should be noted that this simulation involves some unverified assumptions; it cannot be considered a validation of the code.

The code is limited to flow only and cannot treat a fully three-dimensional problem. Results from this code are generally accepted as being valid and correct, when the code is properly applied.

References -

1. A.E. Reisenauer, "Variable Thickness Transient Groundwater Flow Model (VTT), Formulation, User's Manual and Program Listings," Pacific Northwest Laboratory Report PNL 3160-1, PNL 3160-2, PNL 3160-3, 1979.

2. S.K. Gupta, C.R. Cole, and F.W. Bond, "Finite Element Three Dimensional Groundwater (FE3DGW) Flow Model, Formulation, Program Listings and User's Manual," Pacific Northwest Laboratory Report PNL-2939, 1979.

3. Kellogg, O.C., Foundations of Potential Theory, Dover, New York, 1954 .

2.6 V3 Area: Repository Siting

I. Summary of Code

Purpose and Scope - This series of finite-difference models was developed to simulate ground-water flow under a variety of flow conditions.

Authors - V3 was developed at the Illinois State Water Survey and is described in a bulletin by T.A. Prickett and C.G. Lonnquist.

Code Functions - 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 ground-water reservoir, the process of ground-water evapotranspiration, the mechanism of possible conversion of storage coefficients from artesian to water-table conditions, and the multiple-aquifer problem.

Potential Usage - This code was designed to simulate a variety of ground-water flow conditions within an aquifer system. V3 may be used to examine conditions in the regional area.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - V3 is available to the public. In general, the documentation, which is obtained from the Illinois State Water Survey (ref. 1), contains listings of the codes. The programs are relatively short and can be punched using the listings.

II. Summary of Findings

General Critique - V3 is one of the most widely used ground-water flow codes. The code is well documented, has been fully debugged, and has been field verified. In addition, it offers many options in terms of flow conditions and recharge/discharge.

Perhaps the best way to critique V3 is by way of comparison with the U.S. Geological Survey codes. In V3, the approach to model programming is fundamentally different from the approach used in USGS2D and USGS3D. Rather than having one comprehensive program, V3 represents a series of models that can be used for different applications. This approach has some distinct advantages:

- Simple models can be used for simple problems and complicated models for complex problems.
- The programs are shorter and easier to understand.
- The programs are easy to modify.

The disadvantages of V3 include:

- It is necessary to maintain many different programs.
- Program modifications are often necessary.
- Only steady-state leakage is considered.
- Only one matrix solution technique (iterative alternating direction implicit) is provided. This could result in convergence difficulties for certain field problems.
- There is no check on mass balance.
- A separate node property card is required for each node when variable grid spacing is used.

Applicability to Medium - V3 is designed for most types of geological media where flow in a porous medium can be assumed.

Sensitivity Analysis - Numerous sensitivity calculations have been performed with this code. These sensitivity calculations include both numerical and physical parameters for specific problems. The numerical parameters include (1) matrix solution technique, (2) matrix parameters such as overrelaxation parameters, (3) grid spacing, and (4) time steps. Physical parameters that have been varied include (1) hydraulic conductivity, (2) storage properties, (3) leakage properties, and (4) recharge properties.

Code Verification - V3 has been compared to several analytical solutions, including those by Theis, Hantush and Jacob. It does not contain a mass balance.

Field Validation - This code has been applied extensively to field problems. The documentation includes results from an application to a Cambrian-Ordovician aquifer in northeastern Illinois. Another example of a field application is given in ref. 2, where the code was used to examine a waste-water disposal site in Muskegon County, Michigan. Most of the applications have dealt with water supply problems associated with relatively shallow aquifers.

III. General Description

Operating Characteristics - 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.

V3 is programmed in a 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.

Inputs - Input for the basic aquifer simulation program includes:

Parameter and default value cards
Array data
Transmissivity
Storage coefficient
Initial hydraulic heads
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 area of the streambed
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

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

Available Documentation - Documentation (ref. 1) for V3 may be obtained from Illinois State Water Survey, Urbana, Illinois 61801.

IV. Review of Theory

Equations - The partial differential equation (considered in the basic aquifer simulation program) of ground-water flow in a confined aquifer in two dimensions, where it is assumed that the cartesian coordinate axes are aligned with the principal components of the transmissivity tensor, may be written as

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y}\right) = S \frac{\partial h}{\partial t} + W(x,y,t) \qquad (2.48)$$

where

T_x, T_y are the principal components of the transmissivity tensor (L^2t^{-1});
h is hydraulic head (L);
S is the storage coefficient (dimensionless);
W is the volumetric flux of recharge or withdrawal per unit surface area of the aquifer (Lt^{-1}).

Numerical Approximation - Equation (2.48) is solved using a finite-difference approximation. Whereas the U.S. Geological Survey codes derived the finite-difference equations by a conventional mathematical treatment, the approach in V3 is to develop the finite-difference equations from a physical standpoint involving Darcy's equation and the principle of conservation of mass. The grid used in this approach may be variable and is lattice centered; that is, the nodes are located at the block intersections.

The matrix equation is solved by a modified alternating direction implicit procedure. For this procedure, a set of finite-difference equations are solved by columns and then another set of equations is solved by rows. The column equations may be written as follows:

$$AA_j\, h_{i,j-1} + BB_j\, h_{i,j} + CC_j\, h_{i,j+1} = DD_j \tag{2.49}$$

where the constant terms are

$$AA_j = -T_{i,j-1,x} \tag{2.50}$$

$$BB_j = T_{i-1,j,y} + T_{i,j,y} + T_{i,j,x} + T_{i,j-1,x} + S\Delta x^2/\Delta t \tag{2.51}$$

$$CC_j = -T_{i,j,x} \tag{2.52}$$

$$DD_j = (S\Delta x^2/\Delta t)\hat{h}_{i,j} + W_{i,j} + T_{i-1,j,y}h_{i-1,j} + T_{i,j,y}h_{i+1,j} + W_n \tag{2.53}$$

The row equations may be written as:

$$AA_i h_{i-1,j} + BB_i h_{i,j} + CC_i h_{i+1,j} = DD_i \tag{2.54}$$

where the constant terms are

$$AA_i = -T_{i-1,j,y} \tag{2.55}$$

$$BB_i = T_{i-1,j,y} + T_{i,j,y} + T_{i,j,x} + T_{i,j-1,x} + S\Delta x^2/\Delta t \tag{2.56}$$

$$CC_i = -T_{i,j,y} \tag{2.57}$$

$$DD_i = (S\Delta x^2/\Delta t)\hat{h}_{i,j} - W_{i,j} + T_{i,j-1,x}h_{i,j-1} + T_{i,j,x}h_{i,j+1} + W_n \tag{2.58}$$

where Δx and Δy are the spacing in the x- and y-directions, respectively, i and j are the counters in those respective directions, Δt is the time step, and $\hat{h}$ is the head from the previous time step.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The major assumptions are as follows:

- 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

Structure and Level of Detail - 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, source term options, and solution techniques.

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

Applicability, Limitations, Validity, and Completeness - The program can treat most anticipated flow conditions. Results of this code are widely accepted as being valid and correct, when the code is properly applied. However, lack of a mass balance is a disadvantage.

References -

1. Prickett, T.A. and C.G. Lonnquist, "Selected digital computer techniques for groundwater resource evaluation," Illinois State Water Survey, Bulletin 55, 1971

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

3.0 UNSATURATED FLOW CODES

3.1 FEMWATER Area: Repository Siting

I. Summary of Code

Purpose and Scope - FEMWATER (A Finite-Element Model of Water Flow through Saturated-Unsaturated Porous Media) was developed to simulate ground-water dynamics in saturated-unsaturated subsurface systems.

Authors - FEMWATER 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.

Code Functions - FEMWATER is a two-dimensional finite-element model of water flow through porous media which simulates ground-water dynamics in saturated-unsaturated subsurface systems. The response of the ground-water basin to the rainfall, artificial withdrawal, and other recharge or discharge sources (such as lakes, reservoirs, and streams) may be included in the simulation.

The aquifer to be modeled may be given an areal description or may be cross-sectional. Aquifer parameters may be distributed or zoned and the system may be anisotropic. The model considers nonlinearities by allowing the storage term and the hydraulic conductivity to be a function of the pressure head. Three types of boundary conditions are considered; they all may be functions of time. Additionally, the flow field is computed in a manner consistent with the finite-element approach, thus obtaining continuity of the velocities at the nodes of the finite-element mesh.

Potential Usage - If a site is selected in a deep (or shallow) unsaturated zone, FEMWATER would be of use.

The model is capable of performing a two-dimensional simulation of an aquifer system. This system may have regions of unsaturated or saturated porous media. FEMWATER produces not only a continuous pressure distribution, but also a continuous velocity field. This continuous velocity field is used as input to the companion code, FEMWASTE, which simulates the contaminant transport in such a medium.

FEMWATER is considered a far-field code in the sense that the flow is analyzed outside the disturbed zone.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - The code is in the public domain and is therefore available to the NRC.

II. Summary of Findings

General Critique - The physics of flow in the unsaturated zone is less fully understood than that for flow in the saturated zone. This code is based on state-of-the-art research and is probably about as good as is possible given the present level of understanding.

The model analyzes an aquifer from a plane cross-sectional or areal viewpoint. However, radial coordinates have not been implemented; this would be a major disadvantage in the analysis of radial flow to a well.

FEMWATER is an extension of the work performed by Duguid and Reeves (ref. 2) in which the continuity equation of water mass governing the distribution of pressure head is solved by the Galerkin finite-element method subject to appropriate boundary and initial conditions. In the original Duguid-Reeves code, the flow field is computed directly from Darcy's law by taking the derivatives of the calculated heads. Inherent in that approach, however, is the resulting discontinuity in the velocity at element boundaries and nodal points, which unfortunately leads to a violation of the conservation of mass in a local sense. When the spatial distribution of the velocity is significant in the region, inputting this discontinuous flow field to the contaminant transport computation could conceivably produce a large error. FEMWATER incorporates a technique to overcome this problem by solving Darcy's law for the velocity field at nodal points by the finite-element method rather than by taking the derivatives of the pressure field. This approach is consistent with the spirit of finite-element methods, and yields a continuous velocity over the whole region of interest, including element boundaries and nodal points.

Applicability to Medium - FEMWATER is designed to simulate saturated or unsaturated water flow subject to variable boundary or initial conditions. The code is applicable to most porous media as long as vertical or horizontal averaging is valid and a two-dimensional simulation is performed.

Sensitivity Analysis - A comparison of velocity components simulated by the original code by Duguid and Reeves (ref. 2) to FEMWATER was performed. Unique velocity fields are obtained by the revised model, while the discontinuous velocity fields at all nodal points are obtained by the old model. The discontinuity ranges from several hundred percent to negligible. The overall mass loss through boundaries for the transient problem is reduced from 23.8 percent in the original code to 2.2 percent in FEMWATER for one case and from 29.7 to 3.6 percent for another case.

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 (ref. 1).

Field Validation - None.

III. General Description

Operating Characteristics - FEMWATER is written in FORTRAN for use on an IBM 360 machine.

Inputs - Inputs for FEMWATER include:

Grid geometry
Initial heads
Prescribed head and flux boundary conditions
Hydraulic-conductivity tensor
Modified storage coefficient
Material nonlinearities

Outputs - Output for FEMWATER consists of the pressure distribution and velocity field at each time step.

Available Documentation - FEMWATER is documented in Ref. 1.

IV. Review of Theory

Equations - The governing equations to describe the pressure field in a two-dimensional subsurface system are obtained from the principle of conservation of mass and Darcy's law. This can be written in the form:

$$L(h) = F \frac{\partial h}{\partial t} - \left[\frac{\partial}{\partial x}\left(K_{xx} \frac{\partial H}{\partial x} + K_{xz} \frac{\partial H}{\partial z}\right) + \frac{\partial}{\partial z}\left(K_{zx} \frac{\partial H}{\partial x} + K_{zz} \frac{\partial H}{\partial z}\right)\right] - Q = 0 \tag{3.1}$$

subject to

$$h = h_1(x,z,t) \text{ on } B_1 \tag{3.2}$$

$$- \left[\left(K_{xx} \frac{\partial h}{\partial x} + K_{xz} \frac{\partial h}{\partial z} + K_{xz}\right) \cdot n_x + \left(K_{zx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z} + K_{zz}\right) \cdot n_z\right] = q_2 \text{ on } B_2 \tag{3.3}$$

and

$$h = h_3(x,z,t) \text{ on } B_3 \tag{3.4}$$

or

$$- \left[\left(K_{xx} \frac{\partial h}{\partial x} + K_{xz} \frac{\partial h}{\partial z} + K_{xz}\right) \cdot n_x + \left(K_{zx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z} + K_{zz}\right) \cdot n_z\right] = q_3 \text{ on } B_3 \tag{3.5}$$

where

$$F = \frac{\theta}{\phi}\,\alpha' + \beta'\,\theta + \frac{d\theta}{dh},$$

and

$$H = h + z,$$

in which h is the pressure head; θ is the moisture content; ϕ is the effective porosity; α' and β' are the modified coefficients of compressibility of the medium and water, respectively; K_{xx}, K_{xz}, K_{zx}, and K_{zz} are the hydraulic conductivity tensor components; x and z are the horizontal and vertical coordinates, respectively; t is the time; Q is the artificial recharge or withdrawal; and L is an operator.

Three types of boundary conditions are considered in the problem. In the first type (Dirichlet) boundary, the pressure head is prescribed on B_1 where B_1 is a portion of the boundary B, and h_1 is a known function of time and (x,z) on B_1.

In the second type (Neumann) boundary, the flux is prescribed on B_2 where n_x and n_z are the directional cosines of the outward unit vector normal to the B_2 portion of the curve B.

The third type is the variable in the sense that either the Dirichlet or the Neumann conditions may prevail, where h_3 and q_3 are two known functions of time and (x,z) on the B_3 portion of B. The boundaries, B_1, B_2, B_3, and the impervious boundary, B_I, constitute the entire boundary, B(x,z) = 0. Initially, Equation (3.5) is applied to the boundary B_3 when the exact boundary conditions cannot be predicted a priori. Such a case would arise at the ground surface where either ponding (Dirichlet) or infiltration (Neumann) conditions could prevail. This can only be determined in the cyclic process of solving Equation (3.1).

In general, Equation (3.1) is nonlinear as both the soil properties, F, and hydraulic conductivity, K, are functions of the pressure head.

The initial condition of Equation (3.1) is assumed to be known as:

$$h = h_o(x,z) \text{ in } R, \qquad (3.6)$$

where h_o is a known function of spatial coordinates x and z. R is a region bounded by the curve B(x,z). The function h_o may be obtained by simulating the steady state version of Equation (3.1) with time-invariant boundary conditions.

After Equation (3.1) is solved for the pressure head, h [subject to initial and boundary conditions, Equations (3.2) through (3.6)], the velocity components are then obtained from

$$V_x = -(K_{xx} \frac{\partial h}{\partial x} + K_{xz} \frac{\partial h}{\partial z} + K_{xz}) \quad (3.7)$$

and

$$V_z = -(K_{zx} \frac{\partial h}{\partial x} + K_{zz} \frac{\partial h}{\partial z} + K_{zz}) \quad (3.8)$$

Numerical Approximations - Equations (3.1) through (3.6) are solved by the Galerkin finite-element method. The region of interest is subdivided into an assemblage of smaller subdomains called elements. The quadrilateral bilinear element is used. Following the standard procedure of the Galerkin finite-element method, an approximate formulation of the pressure head h is obtained.

Finite-difference methods are used in the approximation of the time derivative. Three time-marching methods are adopted. In the first one, the central or Crank-Nicholson formulation is used, in which the required matrices are evaluated at $t + \Delta t/2$. In the second method the backward difference formulation is used in which the required matrices are evaluated at $t + \Delta t$. In the third optional method, the values of the unknown variables are assumed to vary linearly with time during the time interval Δt. In this mid-difference method, the required matrices are all evaluated at $t + \Delta t/2$. This option has been shown superior to the central or backward-difference formulation, if the mass matrix is not lumped.

It is important to note that the model also applies the Galerkin technique to Darcy's law so as to produce a continuous flow field. This avoids discontinuities of the flow field at the nodes.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The main assumptions are:

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

Structure and Level of Detail - FEMWATER models an aquifer either from an areal viewpoint or as a cross section. The domain is discretized using four-noded isoparametric finite elements of almost any quadrilateral shape. The time domain is discretized by finite-difference techniques.

Major Dependent Variables - Aside from the input parameters, the major variable is the hydraulic head.

Applicability, Limitations, Validity and Completeness - This code is applicable to both saturated or unsaturated flow in a porous medium. This has evident advantages over codes that only model saturated flow. The code seems to be limited to plane two-dimensional flow, as it does not seem that the radial flow problem has been implemented.

References -

1. G.T. Yeh and D.S. Ward, "FEMWATER: A finite-element model of water flow through saturated-unsaturated porous media," Oak Ridge National Laboratory Report ORNL-5567, 1979.

2. M. Reeves and J.O. Duguid, "Water movement through saturated-unsaturated porous media: A finite-element Galerkin model," Oak Ridge National Laboratory Report ORNL-4927, 1976.

3.2 UNSAT 2 Area: Repository Siting

I. Summary of Code

Purpose and Scope - UNSAT 2 was developed for solving problems of nonsteady seepage in saturated-unsaturated porous media.

Authors - UNSAT 2 was developed at Technion, Israel Institute of Technology, by S.P. Neuman, R.A. Feddes, and E. Bresler.

Code Functions - 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.

Potential Usage - UNSAT 2 is considered a far-field code in the sense that the flow is analyzed outside the disturbed zone.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, 40.

Restrictions - The code is in the public domain and is therefore available to the NRC.

II. Summary of Findings

General Critique - Program UNSAT 2 is an improved and ex[illegible] version of program UNSAT 1 previously developed by Neuman (ref. [illegible]). It utilizes the Galerkin method in conjunction with a finite element discretization scheme for solving problems of nonsteady seepage in saturated-unsaturated porous media.

UNSAT 2 is very flexible in modeling various shaped domains. This is due to the fact that one of three coordinate systems may be adopted (x-y cartesian, x-z cartesian, and r-z cylindrical) and that the boundary of the flow domain may be well matched using triangular elements.

The code has been well tested and seems to perform well when matched against other numerical solutions and experimental field results alike.

Applicability to Medium - UNSAT 2 is designed to simulate saturated/unsaturated water flow subject to variable boundary or initial conditions. The code is applicable to most porous media as long as vertical, horizontal, or cylindrical averaging is valid and a plane two-dimensional or an axisymmetric two-dimensional simulation is performed.

Sensitivity Analysis - Unknown.

Code Verification - Due to the lack of analytic solutions to problems of flow in the unsaturated zone at the time UNSAT 2 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, UNSAT 2. The results were compared.

Field Validation - Two field problems were simulated by UNSAT 2 as reported in Ref. 1. These are: (1) a field experiment performed by Feddes (ref. 2) at the ground-water 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).

III. General Description

Operating Characteristics - UNSAT 2 is written in FORTRAN IV for use on an IBM 370/165 machine.

Inputs - Inputs for UNSAT 2 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
Storage coefficient

Outputs - 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 had 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.

Available Documentation - UNSAT 2 is documented in Ref. 1.

IV. Review of Theory

Equations - The flow of water in a slightly compressible unsaturated or partly-saturated soil can be described by Neuman (ref. 7)

$$L(\psi) = \frac{\partial}{\partial x_i}\left[K^r(\psi)K^s_{ij}\frac{\partial \psi}{\partial x_j} + K^r(\psi)K^s_{i3}\right] - \left[C(\psi) + \beta S_s\right]\frac{\partial \psi}{\partial t} + S = 0 \tag{3.13}$$

where L is a quasilinear differential operator defined in the flow region, $x_i (i=1,2,3)$ are spatial coordinates (x_3 the vertical), K^r is relative hydraulic conductivity ($0 \leq K^r \leq 1$), K^s_{ij} is conductivity tensor at saturation, ψ is pressure head, C is specific moisture capacity (defined as $\partial\theta/\partial\psi$), β is 1 in the saturated zone and 0 in the unsaturated zone, S_s is specific storage (defined as the volume of water instantaneously released from storage per unit bulk volume of saturated soil when ψ is lowered by one unit), t is time, and S is a positive sink term (or, equivalently, a negative source term). In our case, S represents the volume of water taken up by the roots per unit bulk volume of the soil in unit time.

The quantities K^s_{ij} and S_s are functions of position only. The term S_s reflects the combined elastic properties of the medium and the water when one is willing to assume that lateral strains are negligible and that the total stress at each point remains fixed in time. In the present work is is assumed that S_s can be disregarded in the unsaturated zone because the effect of compressibility on the storage of water is negligibly small in comparison to the effect of changes in the moisture content, θ.

The pressure head, ψ, is taken to be positive in the saturated zone and negative in the unsaturated zone. In the absence of hysteresis, K^r and ψ are monotonically increasing single-valued functions of θ, and C is the derivative of θ with respect to ψ.

According to Feddes et al. (ref. 4), the sink term can be expressed as

$$S = K^r K^s_{11} (\psi - \psi_r) b' \tag{3.14}$$

where ψ_r is pressure head in the roots and K^s_{11} is principal conductivity parallel to the horizontal (x_1) axis (all diagonal components of K^s_{ij} are implicitly assumed to be zero in the root zone). The term b' is an empirical quantity referred to herein as root effectiveness function. Assuming that the rate of uptake by roots is proportional to the pressure head gradient across the soil-root interface, as well as to the cross-sectional area of the flux, it is then evident that b' must represent the ratio between the specific surface area of the roots and the impedance (thickness divided by conductivity) of the soil-root interface.

Equation (3.13) must be supplemented by appropriate initial and boundary conditions. As hysteresis is not considered in the present work, ψ is a single-valued function of θ and, therefore, the initial conditions are simply

$$\psi(x_i, 0) = \Psi_o(x_i) \tag{3.15}$$

where Ψ_o is a prescribed function of x_i. In addition to this, one must specify either the pressure head or the normal flux at each point along the boundary. If Γ_1 is the segment of the boundary, Γ, along which pressure heads are prescribed, and Γ_2 is the complementary segment of Γ along which normal fluxes are prescribed (such that $\Gamma = \Gamma_1 \cup \Gamma_2$), then the boundary conditions become:

$$\psi(x_i, t) = \Psi(x_i, t) \quad \text{on} \quad \Gamma_1 \tag{3.16}$$

$$K^r\left(K^s_{ij} \frac{\partial \psi}{\partial x_j} + K^s_{i3}\right) n_i = -V(x_i, t) \quad \text{on} \quad \Gamma_2 \tag{3.17}$$

Here Ψ and V are prescribed functions of x_i and t, and n_i is the unit outer normal vector on Γ.

Along soil-air interfaces, the exact boundary conditions to be assigned at the soil surface cannot be predicted a priori, and a solution must be sought by maximizing the absolute value of the flux (while maintaining the appropriate sign) subject to the requirements (see Hanks et al., ref. 5).

$$| K^r (K^s_{ij} \frac{\partial \psi}{\partial x_j} + K_{i3}) n_i | \leq | E^*_s |$$

(3.18)

$$\psi_L \leq \psi \leq 0$$

where E^*_s is the prescribed potential surface flux (positive when directed into the system as in infiltration, and negative when directed out of the system as in evaporation) and ψ_L is the minimum allowed pressure head at the soil surface. Both E^*_s and ψ_L may vary with time.

A seepage face is another kind of atmospheric boundary at which water seeps out from the saturated portion of a porous medium. The length of the seepage face varies with time in a manner that can never be predicted a priori. On the other hand, pressure head along the seepage face must be uniformly zero (as atmospheric pressure is also taken to be zero).

Numerical Approximations - Equations (3.13) through (3.18) are solved by the Galerkin method in conjunction with a finite-element discretization scheme. The flow region is subdivided into a network of elements. It is convenient to adopt a network composed of triangular elements for plane flow and a network composed of concentric rings of constant triangular cross section for axisymmetric problems.

The time domain is discretized into a sequence of finite intervals, t, and the time derivatives are replaced by finite differences. If the entire flow system remains unsaturated at all times, good results can be obtained by employing a time-centered scheme. If part of the system is saturated and S_s in this part is zero, the governing equations in this zone become elliptic. This means that sudden changes in boundary conditions around the saturated zone have an instantaneous effect on the values of ψ everywhere in this zone and ψ is no longer a continuous function of time. To overcome this problem, a fully implicit backward difference scheme in terms of ψ is adapted.

Probabilistic of Statistical Aspects - None.

Assumptions and Simplifications - The main assumptions are:

- Darcy's law is valid and hydraulic-head gradients are the only significant driving mechanisms 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.
- The relative permeability and capillary pressures are functions of moisture content.

Structure and Level of Detail - UNSAT 2 may model a soil system from an areal viewpoint or as a plane or axisymmetric cross section. The domain is discretized using three-noded triangular elements. The time domain is discretized by finite-difference techniques.

Major Dependent Variables - Aside form the input parameters, the major variable is the pressure head.

Applicability, Limitations, Validity and Completeness - This code is applicable to both saturated or unsaturated flow in a porous medium. This has evident advantages over codes that only model saturated flow. To be sure, saturated flow codes have the advantage of being less complicated and more computationally efficient.

References -

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

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

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

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

5. Hanks, R.J., Klute, A. and Bresler, E., "A numeric method for estimating infiltration, redistribution, drainage, and evaporation of water from soil," Water Resources Research, Vol. 5, No. 5, pp. 1064-1069, 1969.

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

7. Neuman, S.P., "Saturated seepage by finite elements," Proc. ASCE, J. Hydraul. Division, Vol. 99, No. HY12, pp. 2233-2250, 1973.

4.0 SURFACE WATER FLOW CODES

4.1 HEC-1 Area: Surface Water Flow

I. Summary of Code

Purpose and Scope - The HEC-1 model is designed to simulate the surface runoff response of a river basin to precipitation or man-made flooding by representing the basin with interconnected hydrologic and hydraulic components. It is primarily applicable to flood simulation.

Authors - HEC-1 was developed at the Hydrologic Engineering Center, Davis, California, by Leo R. Beard.

Code Functions - HEC-1 simulates a stream network using four components: (1) runoff from a subbasin, (2) hydrograph routing, (3) combining of hydrographs, and (4) flow diversion. Most complex branching stream networks can be simulated with the model. The various options for watershed runoff calculation are described, including: precipitation, interception/infiltration, precipitation excess-to-runoff transformation, river routing, and flow through reservoirs. Diversions and multi-stage pumping plant capabilities are also described. Flow in urban areas can be simulated using kinematic wave routing of rainfall excess along a path which includes overland flow elements, collector channels, and a main channel to a subbasin outlet.

Potential Usage - HEC-1 is a mathematical watershed model containing several methods with which to simulate surface runoff and river/reservoir flow in river basins. The hydrologic model together with flood damage computations (also included in the model) provide a basis for evaluation of flood control projects. HEC-1 is most useful for examining conditions in the regional area.

The associated model HEC-2 must be used to obtain the flood profile water surface elevation as a function of location if that is desired.

Related NRC Issues (See Table 1-4) - 22, 24, 27, and 28.

Restrictions - The code is available to the public.

II. Summary of Findings

General Critique - HEC-1 may be useful for examining some of the problems associated with surface flooding. This flooding, which may be due to natural storms or the failure of large-scale man-made surface water impoundments (e.g. dams), may significantly affect the ground-water flow field. Due to the lack of data usually associated with this type of analysis, a detailed model of channel flow is not normally justified. HEC-1 uses a stream network model which can simulate storm flooding and flooding due to dam overtopping and structural failure. The code is commonly used and is well accepted.

Under certain circumstances, flooding of a site area may cause a significant change in the ground-water flow field, affecting the paths taken by the contaminants in question. The analysis of possible flooding and its consequences must be taken into account in repository siting.

Applicability to Medium - HEC-1 is applicable to all surface waters.

Sensitivity Analysis - The literature provides little insight into the sensitivity of the model. The user's manual cautions that care should be exercised when interpreting the results of the dam-break routine. Approximately one percent of the inputs, such as infiltration loss rate, are by judgment, a marked improvement over the five to ten percent for other surface water codes (ref. 5).

Code Verification - Numerous example problems are given in the HEC-1 user's manual. However it is not clear whether these are merely hypothetical problems or actual field problems.

Field Validation - Validation consists of comparing the recorded outflow hydrograph from an actual storm to a hydrograph computed by HEC-1. Ref. 5 and the user's manual provide specific examples where the results are quite good. An overall reliability however is not stated. The HEC-1 package program has been used by government agencies and consulting firms throughout the United States since 1968.

III. General Description

Operating Characteristics - The HEC-1 program, written in FORTRAN IV, requires 350,000 octal words (116,000 decimal) of core storage on a CDC Cyber 175 computer. Disk storage is needed for the 16 output and scratch files used by the program. The program has been operated on CDC and Harris computers.

Inputs - The required data includes:

Hydrograph data
Basin data
Precipitation data
Loss (infiltration data)
Unitgraph data
Snowmelt data
Routing data
Storage data
Diversion data
Pump withdrawal data

Outputs - A large variety and degree of detail in the printer output are available from HEC-1. The degree of detail of virtually all of the program output can be controlled by the user. The output consists of:

- Input data feedback
- Intermediate simulation results
- Summary results
- Error messages

Available Documentation - HEC-1 is well documented in "HEC-1 Flood Hydrograph Package User's Manual" by the U.S. Army Corps of Engineers, Hydrologic Engineering Center, Davis, California, September 1981.

IV. Review of Theory

Equations - As the main objective is to evaluate the effect of flooding, whether natural or man-made, on the ground-water flow patterns, only the equations governing flood routing will be included.

A river basin is subdivided into an interconnected system of stream network components (e.g., Figure 4-1) using topographic maps and other geographic information. A basin schematic diagram (e.g., Figure 4-2) of these components is developed by the following steps:

(1) The study area watershed boundary is delineated first. In a natural or open area this can be done from a topographic map. However, supplementary information, such as municipal drainage maps, may be necessary to obtain an accurate depiction of an urban basin's extent.

(2) Segmentation of the basin into a number of subbasins determines the number and types of stream network components to be used in the model. Two factors affect the basin segmentation: the study purpose and the hydrometeorological variability throughout the basin. First, the study purpose defines the areas of interest in the basin, and hence, the points where subbasin boundaries should occur. Second, the variability of the hydrometeorological processes and basin characteristics affects the number and location of subbasins. Each subbasin is intended to represent an area of the watershed which, on the average, has the same hydraulic/hydrologic properties. Further, the assumption of uniform precipitation and infiltration over a subbasin becomes less accurate as the subbasin becomes larger. Consequently, if the subbasins are chosen appropriately, the average parameters used in the components will more accurately model the subbasins.

(3) Each subbasin is to be represented by a combination of model components. Subbasin runoff, river routing, reservoir, diversion and pump components are available to the user.

(4) The subbasins and their components are linked together to represent the connectivity of the river basin. HEC-1 has available a number of methods for combining or linking together outflow from different components. This step completes the basin schematic.

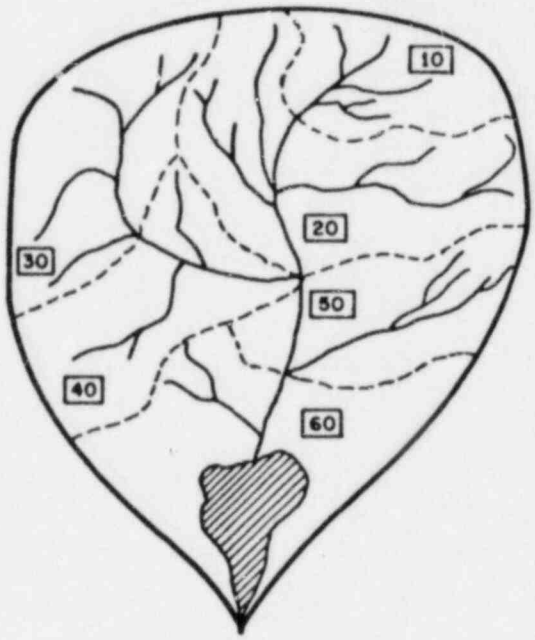


Figure 4-1. Example River Basin

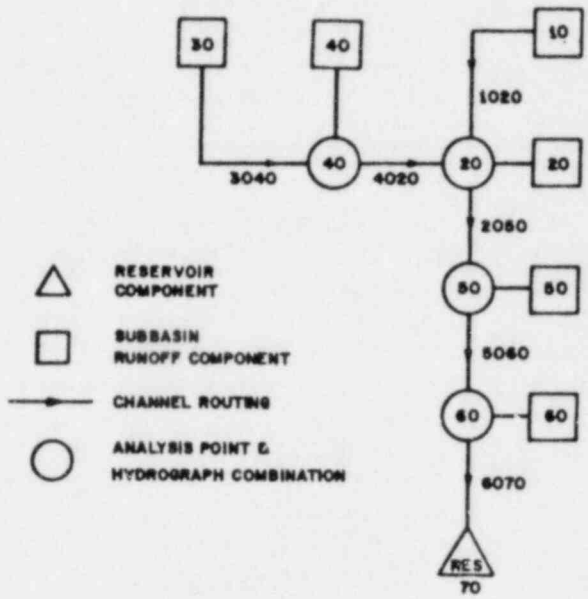


Figure 4-2. Example River Basin Schematic

Flood routing is used to simulate flood wave movement through river reaches and reservoirs. Most of the flood-routing methods available in HEC-1 are based on the continuity equation and some relationship between flow and storage or stage. These methods are Muskingum, kinematic wave, modified Puls, working R and D, and level-pool reservoir routing. In all of these methods, routing proceeds on an independent-reach basis from upstream to downstream; neither backwater effects nor discontinuities in the water surface such as jumps or bores are considered.

Storage routing methods in HEC-1 are those methods which require data that define the storage characteristics of a routing reach or reservoir. These methods are: modified Puls, working R and D, and level-pool reservoir routing.

Channel infiltration losses may be simulated using the following equation:

$$Q(I) = [QIN(I) - QLOSS] * (1-CLOSS) \tag{4.1}$$

where QIN(I) is the inflowing hydrograph ordinate at time I before losses, QLOSS is a constant loss in cfs, CLOSS is a fraction of the remaining flow which is lost, and Q(I) is the hydrograph ordinate after losses have been removed. Hydrographs are adjusted for losses after routing for all methods except modified Puls; for modified Puls losses are computed before routing.

The Muskingum method (ref. 1) computes outflow from a reach using the following equations:

$$QOUT(2) = (CA-CB) * QIN(1) + (1-CA) * QOUT(1) + CB * QIN(2) \tag{4.2}$$

$$CA = \frac{2 * \Delta t}{2 * AMSKK * (1-X) + \Delta t} \tag{4.3}$$

$$CB = \frac{\Delta t - 2 * AMSKK * X}{2 * AMSKK * (1-X) + \Delta t} \tag{4.4}$$

where QIN is the inflow to the routing reach in cfs. QOUT is the outflow from the routing reach in cfs, AMSKK is the travel time through the reach in hours, Δt is the routing interval in hours, and X is the Muskingum weighting factor ($0 \leq X \leq 0.5$). The routing procedure may be repeated for several subreaches (designated as NSTPS) so the total travel time through the reach is AMSKK. To insure the method's computational stability and the accuracy of the computed hydrograph, the routing reach should be chosen so that:

$$\frac{1}{2(1-X)} \leq \frac{AMSKK}{NSTPS * \Delta t} \leq \frac{1}{2X} \tag{4.5}$$

The kinematic wave technique transforms rainfall excess into subbasin outflow. In the kinematic wave interpretation of the equations of motion, it is assumed that the bed slope and water-surface slope are equal and acceleration effects are negligible (parameters given in metric units are converted to English units for use in these equations). The momentum equation then simplifies to

$$S_f = S_o \tag{4.6}$$

where S_f is the friction slope and S_o is the channel bed slope. Thus flow at any point in the channel can be computed from Manning's formula:

$$Q = \frac{1.486}{n} S^{1/2} R^{2/3} A \tag{4.7}$$

where Q is flow (cfs), S is the channel bed slope (ft/ft), R is hydraulic radius (ft), A is cross-sectional area (ft^2), and n is Manning's resistance factor (dimensionless). The equation can be simplified to

$$Q = \alpha A^m \tag{4.8}$$

where α and m are related to flow geometry and surface roughness. Figure 4-3 gives relations for α and m for channel shapes used in HEC-1. Since the momentum equation has been reduced to a simple functional relation between area and discharge, the movement of a flood wave is described solely by the continuity equation

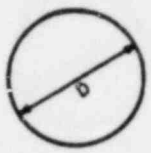
$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q \tag{4.9}$$

where q is the lateral inflow to the channel (L^2/T).

The modified Puls routing method (ref. 2) is a variation of the storage routing method described by Henderson (ref. 3). It is applicable to both channel and reservoir routing. Caution must be used when applying this method to channel routing. The degree of attenuation introduced in the routed flood wave varies depending on the river-reach lengths chosen, or, alternatively, on the number of routing steps specified for a single reach. The number of routing steps (variable NSTPS) is a calibration parameter for the storage routing methods; it can be varied to produce desired routed hydrographs. A storage indication function is computed from given storage and outflow data.

$$STRI(I) = C * \frac{STOR(I)}{\Delta t} + \frac{OUTFL(I)}{2} \tag{4.10}$$

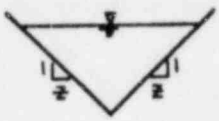
CIRCULAR



$$\alpha = \frac{.804}{n} S^{1/2} D^{1/6}$$

$$m = 5/4$$

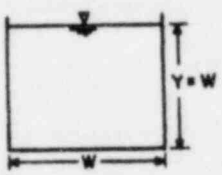
TRIANGULAR



$$\alpha = \frac{0.94}{n} S^{1/2} \left(\frac{z}{1+z^2} \right)^{1/3}$$

$$m = 5/3$$

SQUARE



$$\alpha = \frac{.72}{n} S^{1/2}$$

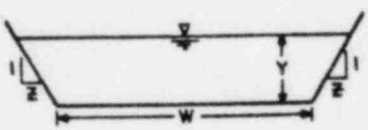
$$m = 4/3$$

RECTANGULAR

$$\alpha = \frac{1.49}{n} S^{1/2} W^{-2/3}$$

$$m = 5/3$$

TRAPEZOIDAL



$$Q = \frac{1.49}{n} S^{1/2} A^{5/3} \left(\frac{1}{W+2Y\sqrt{1+z^2}} \right)^{2/3}$$

Figure 4-3. Kinematic Wave Parameters for Various Channel Shapes

where STRI is the storage indication in cfs, STOR is the storage in the routing reach for a given outflow in acre-ft, OUTFL is the outflow from routing reach in cfs, C is the conversion factor from acre-ft/hr to cfs, Δt is the time interval in hours, and I is a subscript indicating corresponding values of storage and outflow. Storage indication at the end of each time interval is given by

$$STRI(2) = STRI(1) + QIN - Q(1) \tag{4.11}$$

where QIN is the average inflow in cfs, Q is the outflow in cfs, and subscripts 1 and 2 indicate beginning and end of the current time interval.

The outflow at the end of the time interval is interpolated from a table of storage indication (STRI) versus outflow (OUTFL). Storage (STR) is then computed from

$$STR = (STRI - \frac{Q}{2}) * \frac{\Delta t}{C} \tag{4.12}$$

When stage data are given, stages are interpolated for computed storages. Initial conditions can be specified in terms of storage, outflow, or stage. The corresponding value of storage or outflow is computed from the given initial value.

The working R and D method (ref. 1) is a variation of modified Puls method, but accounts for wedge storage as in the Muskingum method. The number of steps and the X factor are calibration parameters of the method and can have a significant effect on the routed hydrograph.

The "working discharge", D, is given by

$$D = X * I + (1-X) * O \tag{4.13}$$

and storage indication, R, is given by

$$R = \frac{S}{\Delta t} \frac{D}{2} \tag{4.14}$$

where I is the inflow hydrograph ordinate, O is the outflow hydrograph ordinate, S is the storage volume in routing reach, and X is the Muskingum coefficient which accounts for wedge storage. The calculation sequence is as follows:

(1) set initial D and R from initial inflow, outflow, and storage

(2) compute R for next step from

$$R_2 = R_1 + \frac{I_1 + I_2}{2} - D_1 \qquad (4.15)$$

(3) interpolate D_2 from R versus D data

(4) compute outflow from

$$O_2 = D_2 - \frac{X}{1-X} * (I_2 - D_2) \qquad (4.16)$$

The storage versus outflow relationship may be specified as direct input or computed by the normal-depth option as described above.

Level-pool reservoir routing assumes a level water surface behind the reservoir. Using the principle of conservation of mass, the change in reservoir storage, S, for a given time period, Δt, is equal to average inflow, I, minus average outflow, O.

$$\frac{S_2 - S_1}{\Delta t} = \frac{I_1 + I_2}{2} - \frac{O_1 + O_2}{2} \qquad (4.17)$$

An iterative procedure is used to determine end-of-period storage, S_2, and outflow, O_2. An initial estimate of the water surface elevation at the end of the time period is made. S_2 and O_2 are computed for this elevation and substituted in the following equation:

$$Y = \frac{S_2 - S_1}{\Delta t} - \frac{I_1 + I_2}{2} + \frac{O_1 + O_2}{2} \qquad (4.18)$$

where Y is the continuity error for the estimated elevation. The estimated elevation is adjusted until Y is within ±1 cfs.

Numerical Approximations - The principal numerical approximations are:

- Averaging of hydraulic/hydrologic properties within each subbasin;
- Averaging of the precipitation and infiltration within each subbasin; and
- Neglect of detailed dynamics of channel flow.

Probabilistic or Statistical Aspects - The principal statistical element is the use of predictions of future storms based on previous rainfall histories.

Assumptions and Simplifications - A river basin is represented as an interconected group of sub-areas. The assumption is made that the hydrologic processes and topographic features can be represented by model parameters which reflect average conditions within a sub-area. These conditions include distribution of precipitation and infiltration capacity, basin and channel slope and roughness, and distribution of snowcover. It would be necessary to consider smaller sub-areas if averages of those parameters are inappropriate for a sub-area. Assumptions inherent in unit hydrograph theory are also present in this model. Some model parameters such as precipitation and infiltration represent temporal as well as spatial averages. Thus the time interval to be used should be small enough that averages over the computation time are applicable. Empirical simplifications of snowmelt and loss rates are utilized. Hydrologic routing techniques simplify the procedure of flood routing.

Structure and Level of Detail - The code is based on subdividing the river basin using topographic maps and other geographic information and representing it as an interconnected system of stream-network components. The stream-network model is the foundation capability of the HEC-1 program. All other computation options build on the stream-network model's capability to calculate flood hydrographs at desired locations in a river basin.

Major Dependent Variables - When considering flooding due to natural causes (i.e. storms) or due to manmade causes (i.e. dam breaks) the required information would be:

- The quantity of water flowing over the surface;
- The quantity of water infiltrating into the ground;
- The paths of the surface-water flow;
- The topographical position of infiltration;
- The time duration of the above.

Applicability, Limitations, Validity and Completeness - There are several important limitations of the model. Simulations are limited to a single storm due to the fact that provision is not made for soil moisture recovery during periods of no precipitation. The model results are in terms of discharge and not stage, although stages can be printed out by the program based on a user-specified rating curve. Streamflow routings are performed by hydrologic routing methods and do not reflect the full St. Venant equations which are required for very flat river slopes. Reservoir routings are based on the modified Puls techniques which are not appropriate where reservoir gates are operated to reduce flooding at downstream locations.

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3. Henderson, F.M., Open Channel Flow, Macmillan, New York, pp. 356-362, 1966.

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5. Viessman, W., Jr., J.W. Knapp, G.L. Lewis, and T.E. Harbaugh, Introduction to Hydrology, Harper & Row, New York, 1977.

4.2 MITCAT Area: Repository Siting

I. Summary of Code

Purpose and Scope - The M.I.T. Catchment Model (MITCAT) is a mathematical computer model for the simulation of storm rainfall and the resulting runoff and streamflow from the land surface.

Authors - MITCAT was developed at the Massachusetts Institute of Technology by J.C. Schaake, Jr., G. Leclerc and B.M. Harley. It is presently maintained and distributed by Camp Dresser and McKee, Inc., Waltham, Massachusetts.

Code Functions - MITCAT is a mathematical watershed model with which to simulate surface runoff and river/reservoir flow in river basins. The main objectives in the development of MITCAT were to produce a computer simulation tool that is easy to use, has practical input-data requirements, and is flexible enough to cover a wide variety of watershed conditions, but still maintains a high degree of accuracy in its results. Specifically, the wide variety of watershed conditions include:

- Precipitation
- Infiltration
- Overland flow
- Channel flow
- Depression storage
- Channel seepage
- Reservoir simulation
- Root zone storage/ground-water storage
- Ground-water outflow

Potential Usage - MITCAT may be used for measuring the hydrologic and hydraulic impacts of urbanization and land-use changes, and the structural and nonstructural controls for mitigating these impacts. It appears, however, that the capability to analyze the effect of dam failure is not present. MITCAT is most useful for examining conditions in the regional area.

Related NRC Issues - (See Table 1-4) - 24, 27, and 28.

Restrictions - The code is available to the public.

II. Summary of Findings

General Critique - MITCAT may be useful for examining some of the problems associated with surface flooding. Flooding due to natural storms may significantly affect the ground-water flow field. Due to the lack of data usually associated with this type of analysis, a rigorous numerical model is not normally required. MITCAT uses a stream network model which has the capability to simulate storm flooding. The code is commonly used and well accepted.

Under certain circumstances, flooding of a site area may cause a significant change in the ground-water flow field, thus affecting the paths taken by the contaminants leaching from a nuclear waste repository. The analysis of possible flooding and its consequences must be taken into account in the repository siting.

The model mainly deals with flooding due to natural storms and the effect that urbanization has on the flood plains and flow channels. It does not appear that MITCAT has the capability to analyze the effect of the possible failure of large-scale man-made surface water impoundments, such as dams. This appears to be a drawback in the application of MITCAT to a system in which failure of such impoundments may be possible in the region of a nuclear waste repository.

Applicability to Medium - MITCAT can handle any catchment of any size or shape, urban or rural, and does not require complex input data to achieve this capability.

Sensitivity Analysis - None reported.

Code Verification - The model was subject to experimental verification (ref. 1).

Field Validation - MITCAT has been widely used throughout the continental United States as well as Puerto Rico and the Philippine Republic. Applications have ranged from drainage studies of small urban areas to development of regional stormwater management policies for urbanizing watersheds. The model has been used particularly in developing urban areas. The U.S. Army Corps of Engineers Hydrologic Engineering Center has recently selected MITCAT as a tool for urban hydrology studies. It has also been adopted by two counties in Virginia to evaluate such problems on a continuing basis. Local planners in Fairfax County (D.C. metropolitan area) and Henrico County (Richmond metropolitan area) now use the model to determine the impacts of new development ranging in scope from proposed 100-acre developments to major zoning changes.

III. General Description

Operating Characteristics - The model is written in FORTRAN IV (extended) and is fully compatible with IBM 360-370, CDC 7600, and Honeywell/Multics machines.

Inputs - The input data to the MITCAT program is based directly on the physical and land-use characteristics of the area being modeled. This includes the required physical data for a contributing area, specification of hydrograph duration, interval and the storm or storms to be simulated.

The required physical data for a contributing area include topographic slopes, estimates of overland flow length and typical surface roughness coefficients (i.e., Manning's "n"), area, and land-use and soil-infiltration information. In order to facilitate the use of existing data, MITCAT allows the user to select from four alternative methods of describing the infiltration process (SCS, API, Holtan or Horton) and from three methods of defining land-use within the study area. Conveyance sections or stream channels are defined by specifying typical cross-sections and roughness estimates plus channel slopes and reach lengths. Again, input requirements are simplified by allowing the user several options for specifying typical "ideal" cross-sections (such as circular, rectangular, trapezoidal, etc.) as well as user-specified "variable" sections. Depending upon the complexity of the desired simulation, the user may also specify base flows, stream rating curves, and/or stream diversions. In the majority of cases, the data collection effort for even complicated hydrologic/hydraulic situations may be limited to direct measurement from topographic and soil survey maps along with minimum field inspections.

Outputs - Given the strength, position and duration of precipitation, the value, area and duration of the following are given as output:

- Infiltration
- Overland flow
- Channel flow
- Reservoir/lake storage

Additionally,

- MITCAT can scan outflow hydrographs to see if present values of discharge/stage/velocity are exceeded at design points.
- Printed, plotted hydrographs can be displayed.
- Hydrographs can be stored in disk files for future retrieval and analysis.
- Summary tables of peak discharge, stage, etc., are generated.

Available Documentation - Documentation is available for MITCAT and may be obtained from Dr. B.M. Harley, Camp Dresser and McKee, Inc., 235 Wyman Street, Waltham, Massachusetts.

IV. Review of Theory

Equations - The MITCAT modeling scheme is based upon the philosophy that a highly detailed representation of the movement of water over the very irregular land surface is neither possible nor necessary. Rather, the natural complexities have been reduced to a number of simple elements such as overland flow planes, stream segments, pipe lengths and reservoirs. Flow through such elements is represented with mathematical relations derived from hydraulic principles and solved with proven numerical techniques. By assembling a number of elements, the user can construct a simplified model of an actual watershed. This model eliminates unnecessary details of the actual catchment, but preserves the aggregate characteristics which have significant effects upon the runoff and stream flow behavior. Such a construction is shown for an example catchment in Figure 4-4.

The equations chosen to represent overland flow and stream flow were derived from the partial differential equations for unsteady flow in open channels. The resulting form of these equations is known as the kinematic wave equation.

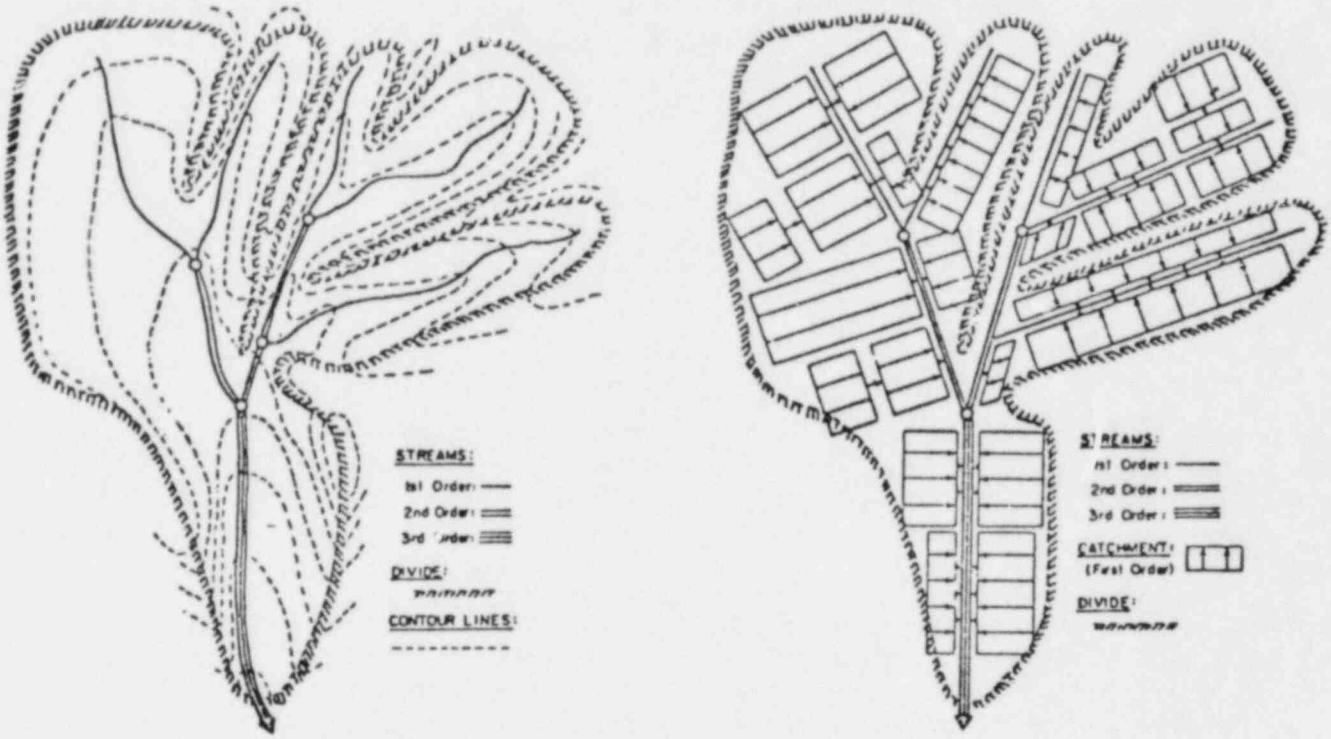
As the important characteristic of overland flow is that the water is distributed over a wide area at a very small average depth until it reaches a well-defined stream channel, the kinematic wave equation for an overland flow segment is

$$\frac{\partial y}{\partial t} + \frac{\partial q}{\partial x} = (i - f)/43200 \qquad (4.19)$$

$$q = \alpha_c y^{m_c} \qquad (4.20)$$

where y is the depth of flow (ft), q if the rate of flow (cfs/ft), t is time (sec), x is distance along the segment (ft), i is the rainfall intensity (in/h)] and f is the infiltration rate (in/hr). In Equation 4.19 both i and f may vary with x and t. The difference i - f may be treated as an effective rainfall rate (which by convention in hydrology is never negative), or the water remaining on the surface when f exceeds i may be permitted to continue to percolate into the soil. The fact that f may vary with x causes the model to simulate runoff only from those locations where i exceeds f.

For modeling of the stream segments, many routing techniques are available, ranging from solutions of the full non-linear continuity and momentum equations through progressively simplified or linearized forms of these equations to simple parametric storage models. It would be desirable to use a form of these equations which is compatible with the overland flow model requirements and which would represent those nonlinearities important to the dynamic behavior of the catchment.



A. B.

Figure 4-4. Representation of Actual Catchment (A) in MITCAT (B)

Using the assumption that the kinematic wave is dominant in the stream flow, thus implying a low Froude number, the corresponding equation for the stream segments is

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q \tag{4.21}$$

$$Q = \alpha_s A^{m_s} \tag{4.22}$$

where A is the cross-section area of flow (ft^2), Q is the discharge rate (cfs) and q is the lateral inflow rate of overland flow (cfs/ft). The above kinematic wave equations contain the parameters, α_c, m_c, α_s and m_s which may be estimated from the Manning formula for the case of overland flow or flow in a triangular channel, respectively (ref. 2).

Numerical Approximations - The principal numerical approximations are:

- Averaging of hydraulic/hydrologic properties within each subbasin;
- Averaging of the precipitation and infiltration within each subbasin; and
- Neglect of detailed dynamics of channel flow.

Probabilistic or Statistical Aspects - The principal statistical element is the use of predictions of future storms based on previous rainfall histories.

Assumptions and Simplifications - A catchment area is represented as an interconnected group of subareas or runoff elements. The assumption is made that hydrologic processes and topographic features can be represented by model parameters which reflect average conditions within an element. These conditions include distribution of precipitation and infiltration capacity, channel slope, and roughness. If such averages are inappropriate for a subarea, then it would be necessary to consider smaller subareas within which average parameters could be used. Model parameters such as precipitation and infiltration represent temporal as well as spatial averages. Thus, the time interval to be used should be small enough that averages over the computation time are applicable.

It has been shown (ref. 3) that the fluid mechanics of flood movement may be separated into the effects of dynamic and kinematic waves, both of which are initially present.

Use of the kinematic form of the unsteady flow equations allows particularly simple numerical solutions (since all disturbances propagate only in the downstream direction), while retaining some of the non-linear effects of the full dynamic form.

As stated by Woolhiser and Liggett (ref. 4), MITCAT assumes that the dynamic effects may be neglected, provided that

$$k = \frac{S_o L}{yF^2} > 10 \qquad (4.23)$$

where S_o is the slope of the stream; L, the length; y, the depth of flow; and F is the Froude number.

Structure and Level of Detail - MITCAT represents the physical movement of water over the catchment surface and through the channel network. The model is based on a recognition that surface geometry is extremely irregular and impossible (and unnecessary) to represent in complete detail in either a physical or a mathematical model. A reductionist approach is used to replace the natural complexities with a number of simple elements such as overland flow planes, stream segments, pipe lengths, etc. A suitable combination of an appropriate number of these simple elements is assumed sufficient to model the behavior of an entire catchment, as illustrated in Figure 4-4.

With various considerations (ref. 1), two basic runoff elements were chosen:

1. Flow distributed over the surface of the catchment would be modeled as planes of overland flow. The inputs to an overland flow plane would be spatially-uniform lateral inflow from rainfall, lateral outflow to infiltration and upstream inflow from adjacent overland-flow segments.

2. Flow from the overland-flow planes would be collected by streamflow segments as lateral inflow and then passed downstream to other stream segments. The term stream is used in a generic sense and includes any open or closed form of conveyance.

Major Dependent Variables - The most important variables within each runoff element, which are computed or changed with time are:

- Infiltration
- Depth of Flow
- Rate of Flow

Applicability, Limitations, Validity and Completeness - The chief limitation of this model is that it was designed primarily for simulating the response of small (less than 100 square miles) watersheds. It is used for studies in developing urban areas. Methods of simulating snowmelt or dam failure are not included in this model.

References -

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3. Lighthill, M.J. and G.B. Whitham, "On kinematic waves - I. flood movement in long rivers," Proc. Ry. Soc. London, A, Vol. 229, pp. 281-316, 1955.

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5.0 GEOCHEMISTRY CODES

5.1 PHREEQE

Area: Waste Package
Repository Siting

I. Summary of Code

Purpose and Scope - PHREEQE (pH-redox-equilibrium equations) was developed to model geochemical reactions. PHREEQE can calculate pH, redox potential, and mass transfer as a function of reaction progress.

Authors - PHREEQE was developed by the United States Geological Survey. The program is described in the U.S. Geological Survey, Water Resources Investigations 80-96 by D.L. Parkhurst, D.C. Thorstenson and L.N. Plummer.

Code functions - PHREEQE models geochemical reactions. PHREEQE can be used to simulate several reactions including: (1) addition of reactants to a solution, (2) mixing of two waters, and (3) titrating one solution with another.

Based on an ion pairing aqueous model, PHREEQE can calculate pH, redox potential and mass transfer as a function of reaction progress. The composition of solutions in equilibrium with multiple phases can be calculated. With respect to elements and aqueous species included in the program's data base, the aqueous model (that is, the nature of the solution components) is exterior to the computer code and is completely user-definable.

Potential Usage - The code can be used to calculate the possible reaction paths in ground water near a repository and aid in interpretation of vertical leakage in nearby aquifers. Specifically, it might be used:

- to predict the dissolution of waste packages and waste forms when equilibrium-limited
- to interpret geochemical evidence bearing on the hydrology of a repository site
- to predict changes in ground-water composition which could affect sorption phenomena.

The major utility of reaction-path modeling is analysis of systems that are sufficiently complex that the available analytical data do not permit definition of reactions by mass balance alone. In this case, reactions can be postulated on the basis of chemical, geologic, or hydrologic data and/or intuition. The chemistry of the aqueous phase, and the mass transfer involved in the reactions, can then be simulated and checked for consistency with the available data. In addition to determining mass transfer and aqueous phase speciation, PHREEQE is capable of calculating pH and pE as dependent variables.

Related NRC Issues (See Table J-4) - 18, 41, and 42.

Restrictions - None. The program is available to the public.

II. Summary of Findings

General Critique - The model appears to be complete in including the major chemical reactions affecting the chemistry of flowing ground water through a rock medium. It is one of a smaller family of programs that are capable of following one or more phase boundaries, and calculating pH and pE as dependent variables in the calculations. In the geochemical literature, these programs have largely been outgrowths of the work of Garrels and Mackenzie (ref. 2) and the theory and computer programs developed by Helgeson and co-workers (ref. 5, 6 and 7).

Earlier computer programs for dealing with natural water chemistry such as WATEQ (ref. 11), SOLMNEQ (ref. 8), WATEQF (ref. 10), and WATEQ2 (ref. 1) are designed to calculate solution speciation and saturation states of the aqueous phase with respect to various mineral phases. Analytical concentrations of the elements, pH, temperature and pE (if redox reactions are considered) must be given.

Recent emphasis is being placed on new models (ref. 4) for mixed electrolyte solutions which, although semi-empirical, are based on equally sound thermodynamic foundations. Recent calculations show that some of these models are more successful than the current ion association model used in PHREEQE in highly concentrated solutions such as brines.

One word of caution in using chemical models such as PHREEQE is that a reaction path that models a given set of observed chemical changes is not mathematically unique. That is, the observed changes in water chemistry can often be modeled exactly by two or more reaction paths.

Applicability to Medium - PHREEQE is an extremely general geochemical model and is applicable to most hydrochemical environments. However, it could not be used near a salt repository because it is inapplicable to systems with high brine concentrations.

Sensitivity Analysis - None.

Code Verification - Compared with similar path reaction programs.

Field Validation - None.

III. General Description

Operating Characteristics - PHREEQE is a FORTRAN IV computer program. PHREEQE uses several non-standard IBM FORTRAN H extended enhancements to FORTRAN IV in an effort to conserve memory and shorten the card deck. If the source code is to be used on another computer, the non-standard features may have to be modified. No attempt has been made to give complete statement by statement modifications which might be necessary if problems occur.

Another possible problem in compiling the code on another machine is the ENTRY statement. Two of PHREEQE's subroutines, PTOT and THORIT, are really collections of subroutines which use ENTRY statements instead of SUBROUTINE statements. Each computer handles entry points differently and some do not allow argument lists in the ENTRY statements. In most cases, making each entry point a separate subroutine with all the common blocks and declarations will eliminate any problems.

Inputs - Data requirements are dictated by which one of 10 keywords are selected; refer to pages 25-41 of the documentation.

Outputs - Given the above inputs PHREEQE follows one or more phase boundaries in determining (1) pH, (2) pE (as well as mass transfer and aqueous-phase speciation), (3) the total concentration of elements, (4) amounts of minerals (or other phases) transferred into or out of the aqueous phase, (5) the distribution of aqueous species, (6) and the saturation state of the aqueous phase with respect to specified mineral phases.

Available Documentation - The documentation for PHREEQE is available (ref. 9).

IV. Review of Theory

Equations - PHREEQE was developed to model geochemical reactions between water and rock material. The equations used by PHREEQE are as follows:

(1) Electrical neutrality

$$\sum_{i=1}^{I} z_i \cdot m_i = 0 \qquad (5.1)$$

where z_i is the charge of the ith species and m_i is the molality of the aqueous species.

(2) Conservation of electrons (this equations is only used in determining the speciation in reaction solutions, not initial solutions)

$$\sum_{i=1}^{I} v_i \cdot m_i = OPV + \sum_{p=1}^{P} u_p \cdot Min_p \qquad (5.2)$$

where v_i is the operational valence (OPV) of the aqueous species, m_i is the molality, u_p is the sum of the OPV's of the constituent in the p^{th} mineral and Min_p which is the moles of the p^{th} mineral transferred into (+) or out of (-) the aqueous phase.

(3) Mass balance - the sum of aqueous species equals initial total plus contribution from phases other than aqueous.

$$\sum_{i=1}^{I} c_{i,j} \cdot m_i = TOT_j + \sum_{p=1}^{P} b_{p,j} \cdot Min_p \text{ for each } j \qquad (5.3)$$

where $c_{i,j}$ is the stoichiometric coefficient of the j^{th} master species in the ith aqueous species, TOT_j is the total concentration of the element corresponding to the j^{th} master species preceding any mineral dissolution or precipitation, $b_{p,j}$ is the stoichiometric coefficient of the j^{th} master species in the p^{th} mineral.

(4) Mineral equilibrium (one equation for each mineral phase)

$$\sum_{j=1}^{J} b_{p,j} \cdot \log (a_j) = \log (K_p) \text{ for each } p \qquad (5.4)$$

where a_j is the activity of the j^{th} master species and K_p is the equilibrium constant for the mass action equation for the p^{th} phase.

(5) Mass action equations for the aqueous species

$$\log (a_i) = \log (K_i) + \sum_{j=1}^{J} c_{i,j} \cdot \log (a_j) \qquad (5.5)$$

where a_i is the activity of the ion pair and k_i is the equilibrium constant for the mass action equation.

Numerical Approximations - PHREEQE solves a set of nonlinear algebraic equations using a combination of two iterative techniques and four independent unknowns. The two techniques are:

(1) A continued-fraction approach for mass-balance equations (for estimates of master species),

(2) A modified Newton-Raphson technique for all other equations (for changes in a_{H^+}, a_{e^-}, and mineral transfer).

The four independent unknowns are: (1) a_{H^+}, (2) a_{e^-}, (3) the activity of one aqueous specie for each element, and (4) amounts of mineral mass transfer to the aqueous phase. All other unknowns, activities, activity coefficients, molalities, and the activity of water are calculated from these independent variables.

Probabilistic and Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions are those that are inherent in the chemical equations such as the Debye-Huckel equation (see documentation).

Structure and Level of Detail - PHREEQE is an extremely general geochemical model and is applicable to most hydrochemical environments. The reaction path tested is not necessarily unique and many reaction paths may exist.

Major Dependent Variables - The principal variables of this program are:

- Debye-Hückel equation parameters and constants
- Alkalinity contribution for each species and total alkalinity
- Stoichiometric coefficients
- Electrical imbalances of initial solutions
- Charge difference between the sum of the anions and the sum of the cations
- Temperatures
- Total concentration of elements in solution.

Applicability, Limitations, Validity, and Completeness - PHREEQE is an extremely general geochemical model and is applicable to most hydrochemical environments. Several conceptual and numerical limitations should be considered.

- Water (Masses of H and O) - PHREEQE deals with masses of elements in terms of their concentrations in the aqueous phase and uses electrical neutrality and electron balance relations to complete the set of equations needed to solve a given problem. The masses of H and O are not considered in the numerical solution to the set of simultaneous equations causing errors in the computation. The systems where this can be a problem are:

  Redox systems
  Hydrated minerals
  Evaporation

- Convergence Problems - Due to the non-linear nature of equations involved, the program may not converge on some problems. This is most likely to occur in redox systems.

- Ion Exchange - There are two limitations in the way PHREEQE deals with ion exchange (see documentation).

- Water Stability Limits - Although PHREEQE's calculations are not limited to the stability field for water, convergence problems occur if partial pressures of O_2 and H_2 are greater than one atmosphere.

- Titration and Mixing - A problem occurs because the equations used are valid for volume and molarity or normality, but not for volume and molality. The errors will be proportional to ρ-1, where ρ is the density of the solutions involved in the titration.

- Activity of Water - For numerical purposes PHREEQE has a lower numerical limit of 0.3 imposed to present the activity of water from approaching zero or going negative during intermediate interation steps in which guesses on the sum of the molalities of dissolved anions, cations and neutral species might be very high.

- Uniqueness of Solutions - In many cases in natural systems a reaction or reaction path that models a given set of observed chemical changes is not mathematically unique.

- Brines - The Debye-Huckel model, on which the code is based, breaks down at high ionic strengths. Therefore, the model is inapplicable to brines.

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5.2 EQ3/6

Area: Waste Package
Repository Siting

I. Summary of Code

Purpose and Scope - EQ3/6 was developed to compute equilibrium models of aqueous geochemical systems. The package contains two principal programs. EQ3 performs distribution-of-species calculations for natural water compositions; EQ6 uses the results of EQ3 to predict the consequences of heating and cooling aqueous solutions and of irreversible reaction in rock water systems (ref. 11).

Authors - Most of the work on EQ3/6 was done at the Department of Geological Sciences, Northwestern University. Subsequent work was done at the Lawrence Livermore Laboratory, Livermore, CA. This program is described in the Lawrence Livermore Laboratory Report UCRL-52658 by T.W. Wolery.

Code Functions - EQ3 computes the distribution of chemical species such as ions, neutral species, ion pairs, and complexes in the aqueous solution. This calculation produces a model of the fluid, which specifies the concentration and thermodynamic activity of each chemical species occurring in the chemical system and included in the data base. The program then calculates the saturation state of the fluid with respect to all relevant mineral phases in the data base. The aqueous solution model then acts as a starting point for mass-transfer computations by EQ6 (ref. 11).

EQ6 can be used to compute several mass transfer models. If the initial model fluid is supersaturated with respect to any mineral phases, the program first "equilibrates" it by calculating a new model of modified fluid plus precipitates (ref. 11). EQ6 then computes the reaction progress models of compositional evolution and mass transfer in a closed or open system containing this aqueous solution (ref. 11).

Reaction progress calculated in EQ6 may describe changes in temperature and pressure, irreversible reaction of the fluid with reactants such as rocks, minerals or gases, or both of these simultaneously (ref. 11). The calculation predicts changes in fluid composition, the identity appearance and disappearance of secondary minerals, and the values of reaction progress at which the fluid saturates with reactants. Such computations permit modeling of the effects of heating and cooling aqueous solutions and of irreversible reaction in rock-water systems (ref. 11).

Potential Usage - The major utility of reaction path modeling is analysis of systems that are sufficiently complex that the available analytical data do not permit definition of reactions by mass balance alone. The code might be used:

- to predict the dissolution of waste packages and waste forms when equilibrium-limited

- to interpret geochemical evidence bearing on the hydrology of a repository site

- to predict changes in ground-water composition which could affect sorption phenomena.

Related NRC Issues (See Table 1-4) - 18, 41, and 42.

Restrictions - None. The software is available from the National Energy Software Center.

II. Summary of Findings

General Critique - The code can be used to calculate reaction path chemistry in complex geologic and hydrologic systems such as formation of ore bodies, scaling and plugging in geothermal development, and the long-term isolation of nuclear waste forms.

The model appears to be complete in including the major chemical reactions affecting the chemistry of flowing ground water through a rock medium. In the geochemical literature, these programs have largely been outgrowths of the work of Garrels and Mackenzie (ref. 3) and the theory and computer programs developed by Helgelson and co-workers. One word of caution in using chemical models such as EQ3/6 is that a reaction path that models a given set of observed changes in water chemistry can often be modeled exactly by two or more reaction paths.

A major limitation of EQ3/6 is that the program requires that the pressure either be 500 bars or else be one atmosphere for $T \leq 100$ °C and follow the liquid/vapor equilibrium curve of water for $T \geq 100$ °C.

The first principal program, EQ3, solves the distribution-of-species problem as does similar programs such as SOLSTAT (ref. 6) SOLMNEQ (ref. 7), and WATEQ (ref. 10), and its revised versions, WATEQF (ref. 9) and WATEQ2 (ref. 1).

The second principal program, EQ6, computes models for chemical equilibrium and mass transfer in aqueous systems. Similar programs are PATH1 and PATHCALC (ref. 4; ref. 6). Another reaction path program is PHREEQE (ref. 8).

Applicability to Medium - EQ3/6 is an extremely versatile model and is applicable to most hydrochemical environments including salt.

Sensitivity Analysis - None.

Code Verification - The code was compared with similar path reaction programs in ref. 2.

Field Validation - None.

III. General Description

Operating Characteristics - The total EQ3/6 software package consists of the two principal source codes EQ3 and EQ6, the set of supporting data files, two utility routines for data file management, and sample input files for EQ3 and EQ6 (ref. 11). The package contents are listed in Appendix A of the documentation; the length of the package precludes reproduction of the contents. This software is available from the National Energy Software Center. The EQ3/6 package should be requested on magnetic tape since it consists of over 30,000 card images. All source codes are written in FORTRAN Extended 4.6 language for use on CDC 6600 and 7600 computers. Principal programs EQ3 and EQ6 and utility program EQF each require one or more externals (subroutines) from the International Mathematical and Statistical Library (ref. 11).

Inputs - The input for EQ3 consists of:

- Title
- Temperature (can be variable)
- Density
- Eh or pE
- Convergence limits
- Print options and debugging options
- Electrical neutrality ion (Na^+ or Cl^-)
- Suppressed species (aqueous reactions, minerals, gas, solid solution)
- Species concentrations (molal, molar, mg/l, fugacity, etc.)

The input for EQ6 consists of:

- Title
- Temperature (can be variable)
- Starting and stopping points in reaction progress
- Print intervals (linear and logarithmic)
- Convergence limits
- Reaction step sizes
- Choice of model (no path, titration, closed or flow through)
- Print options and debugging options
- Reactant species (aqueous, mineral, gas, solid or special)
- Concentrations

Outputs - Output for EQ3 contains:

- Listing of species indexing and log K values
- Input constraints
- Suppressed reactions
- Summary of the aqueous phase
- Activity ratios of cations
- Elemental composition of the aqueous phase
- Saturation states of minerals
- Summary of gas fugacities

A pickup deck is written after distribution of species is achieved. It is used as the bottom half of the mass-transfer program, EQ6.

Output for EQ6 contains:

Reactant summary
Element totals for the aqueous phase
Summary of instantaneously precipitated solid phases
Summary of solid phases
Grand summary of solid phases
Mineral saturation state summary

Available Documentation - The documentation for EQ3/6 is available in ref. 11.

IV. Review of Theory

Equations - Not available in documentation but should be basically the same as PHREEQE.

Numerical Approximations - EQ6 uses the Newton-Raphson method to solve the governing equations of chemical equilibrium (which are algebraic rather than differential equations) for a system of specified elemental composition at fixed temperature and pressure (ref. 11). Convergence is aided by optimizing starting estimates and by under-relaxation parameter β where $0 < \beta \leq 1$ and optimizing starting estimates. The minerals present in the stable phase assemblage are found by several empirical methods. Reaction path models may be generated by using this approach in conjunction with finite differences. This method is analagous to applying high-order predictor-corrector methods to integrate a corresponding set of ordinary differential equations, but avoids propagation of error (drift).

EQ6 is a PATH1-like program which used the Newton-Raphson method to solve the system of algebraic equations instead of their counterparts at each stage of reaction progress. This avoids the drift problem mentioned earlier. Taylor's series expressions, based on finite differences, are used to follow the course of the simulation and to predict starting estimates at each new point of the reaction path (ref. 2).

Probabilistic and Statistical Aspects - None.

Major Dependent Variables - The principal variables of this program are:

- Debye-Hückel equation parameters.
- Alkalinity contribution for each species and total alkalinity.
- Stoichiometric coefficients.
- Electrical imbalances of initial solutions.
- Charge differences between the sum of the anions and the sum of the cations.
- Total concentration of elements in solution.

Applicability, Limitations, Validity, and Completeness - EQ3/6 is an extremely flexible geochemical model and is applicable to most hydrochemical environments. Several conceptual and numerical advantages and limitations are listed below:

(1) It avoids problems with the masses of H and O. Wolery (ref. 11) uses mass balance constraints on each element in the system including H and O.

(2) There are certain convergence problems. However, several under-relaxation methods have been used to minimize the problem. One can modify the tolerances used for convergence through the input cards. Divergence is usually indicative of (a) no mathematical solution exists for the assumed set of mineral phases, (b) a bad set of starting estimates, or (c) a poor starting estimate for oxygen fugacity.

(3) No provision has been made in the program for ion exchange.

(4) The program requires that pressure be 1 atmosphere for $T \leq 100°C$ and follow the vapor/liquid equilibrium curve for water when $\overline{T} > 100°C$ or have a constant value of 500 bars for all temperatures.

(5) The model computes reaction paths via three distinct models: (a) titration, (b) closed system, or (c) flow-through (essentially open system), all of which give slightly different results.

(6) The program has the capacity to allow the user to input their own "special reactants", and to modify the data base. This is advantageous if, for example, one wants to use a more realistic encounter with a specific limestone (containing some magnesium) rather than a generalized "calcite".

(7) Apparently, titration and mixing problems do not occur as in PHREEQE.

(8) Can model the mixing of waters via the special reactants input.

(9) Uniqueness of solution - In many cases, in natural systems a reaction or reaction path that models a given set of observed chemical changes is not mathematically unique.

General problems with all reaction-path models are:

(1) No model will be better than the assumptions upon which it is based. Chemical models are based on the ion association approach which creates several problems:
   a. The use of activity coefficient (approximated by semi-empirical equations) to describe the non-ideal behavior of aqueous electrolytes.
   b. In addition, the assumption of ion association may be a naive representation of the true interactions of "ions" in aqueous solutions (Nordstrom et al., 1979).
   c. Inconsistency and inadequacy of activity coefficient equations.

(2) The reliability of the equilibrium constants or free energies used in the model. This can cause large differences in the computed results of models and probably contributes the largest single source of error.

(3) The assumption made about the redox state of aqueous systems. The distribution of redox species depends on what redox potential is assumed to dominate the chemical equilibrium.

(4) The total number of complexes considered by an aqueous model.

(5) Various ways each program handles the carbonate system. The inorganic carbon system of natural waters is usually determined from the titration alkalinity which includes both the carbonate and non-carbonate alkalinity. There is no general agreement as to the precise correction for non-carbonate alkalinity.

(6) Not all of the aqueous models compute temperature corrections.

(7) Every computerized model was developed for somewhat different purposes and there is no general purpose model which can be used for all hydrochemical problems.

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5.3 WATEQF Area: Repository Siting

I. Summary of Code

Purpose and Scope - WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis (ref. 8). The original version was WATEQ written in PL/1 by Truesdell and Jones (ref. 9). The thermochemical data, speciation, activity coefficients, and general calculations procedure of WATEQF is very similar to the PL/1 version.

Authors - WATEQF was developed by U.S. Geological Survey personnel for modeling the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The program is described in the U.S. Geological Water Resources Investigations 76-13 by L.N. Plummer, B.F. Jones, and A.H. Truesdell.

Code Functions - WATEQF calculates the equilibrium distribution of inorganic aqueous species of major and important minor elements in natural waters using chemical analysis and in situ measurements of temperature, pH, and redox potential.

From this model the states of reaction of the water with solid and gaseous phases are calculated. The examination of reaction states may suggest the origin of the dissolved constituents and assist in the prediction of the chemical effects of ground-water production, recharge, and irrigation (ref. 9).

Potential Usage - WATEQF is a general computer program for the calculation of chemical equilibria in natural waters at low temperatures. It may be expanded and updated by the user as additional data on complexes and minerals become available. The code could be used to interpret geochemical evidence bearing on the hydrology of a repository site. If temperatures near a waste canister were held below 100 °C, it might also be used to study waste package performance, waste dissolution, and interactions between backfills and ground water.

Related NRC Issues (See Table 1-4) - 18, 41, and 42.

Restrictions - None. The program is available to the public and can be obtained from the U.S. Geological Survey, National Center, Reston, Virginia.

II. Summary of Findings

General Critique - The code can be used to model the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis.

WATEQF is one of a smaller family of programs that use successive approximation for water equilibria. Garrels and Thompson (ref. 3) were the first to use the method of successive approximation in a hand calculation to solve an equilibrium problem in aqueous geochemistry. This led to development of other models such as WATCHEM (ref. 2) and

Path 1 (ref. 4). The most general first-generation programs of this type are WATEQ (ref. 9); SOLMNEQ (ref. 5) and EQ3 (ref. 11). All three programs have been designed to accept water analyses with on-site values for pH, Eh, and temperature. There is no proton mass balance condition, only mass balances on cations and anions are carried out. WATEQF is an updated more flexible version of WATEQ.

The first concern of aqueous geochemists and solution chemists is to calculate the distribution and activities of species on the assumption that equilibrium exists in the aqueous phase. Species distribution can then be used in several areas of analytical and applied chemistry (ref. 7). Examples include examining the availability of free and reactive ions, testing solubility hypotheses, and determining the potential bioavailability of nutrients or toxic substances. Species distribution also forms the basis for more complex computations involving solutions which change composition by reaction with other solutions and with gases and solids. Equilibrium calculations of this type are particularly helpful in solving interpretive problems encountered in such fields as chemical and environmental engineering, geochemistry, biochemistry, and aquatic ecology (ref. 7).

One word of caution in using chemical models such as WATEQF is that they are only useful if the investigator understands the geologic and hydrologic system. There is a tendency to use these models as ready-made interpretations of a natural system without understanding the weaknesses in the program. These programs and models are usually developed for specific purposes and considered together they represent a wide range of capabilities and features. A detailed comparison of some thirty computerized models is presented by Nordstrom et al. (ref. 7).

Applicability to Medium - WATEQF is a general computer program for the calculation of chemical equilibria in natural waters at low temperatures. It is an expanded version of WATEQ (ref. 9). Manganese speciation has been added to WATEQF and the successive approximation procedure was revised to give much faster convergence. Twenty-one aqueous species and 17 minerals of uranium have been added to WATEQF in a recent modification (ref. 6). The data base for WATEQF has been expanded to include several trace elements in a recent program WATEQ2 (ref. 1). It also includes the advantages of using PL/1 optimizing code with reorganization into several subprogram blocks and the rapid convergence of WATEQF. For a detailed discussion of the capabilities of WATEQF the reader is referred to Plummer et al. (ref. 8).

Sensitivity Analysis - None.

Code Verification - Compared with similar equilibria programs in Nordstrom (ref. 7).

Field Validation - Used widely in field studies.

III. General Description

Operating Characteristics - WATEQF is a FORTRAN IV computer program that models the thermodynamic speciation of inorganic ions and complex species in solution for a given water analysis. The original version (WATEQ) was written in PL/1 program language by A.H. Truesdell and B.F. Jones, (ref. 9). In most cases the thermochemical data, speciation, activity coefficients, and general calculation procedure of WATEQF is identical to WATEQ (ref. 8).

Inputs - The data matrix of species considered and thermochemical constants is read initially, either from disk or cards. The format of the data matrix, the description of input variables, and optional input can be found in Plummer et al. (ref. 8).

Outputs - The output of WATEQF consists of:

1. A table of data constants used in the calculation of the output for each water analysis lists the title card and tabulates most of the input data.

2. After each iteration through the equilibria equations, the difference between the computed and analytical anion species is tabulated.

3. When convergence occurs, various parameters that describe the solution are printed. Examples are ionic strength, activity of water, comparison of computed and analytical charge balance, pH, pE, temperature, P_{CO_2}, P_{O_2}, and total dissolved solids.

4. The concentration of each aqueous species is printed as ppm, molality and activity, and log values, as well as ionic activity coefficients and their logs.

5. Mole ratios and log activity ratios are computed and tabulated.

6. The activity product of 101 minerals and their saturation index, DG_r and log K are printed.

Available Documentation - The documentation for WATEQF is available (ref. 8).

IV. Review of Theory

Equations - WATEQF contains equations for the calculation of:

1. Mass Action Equilibrium

2. Activity Coefficients
   a. The Debye-Hückel Theory
   b. The Mac Innes Assumption

3. Solution of Mass Action and Mass Balance

4. Actjvity Products and Solubility Products

5. Effects of Temperature and Pressure

6. Redox Reactions

7. Gas Partial Pressures

8. Activity of Water

See documentation for detailed explanation.

Numerical Approximation - WATEQF is one of many successive approximation programs for natural water equilibria.

The method of successive approximation has been conveniently described by Wigley (ref. 10) where either a "brute force" method or a "continued fraction" method can be used (ref. 7). The brute force method is the classical approach where mass action expressions are substituted directly into the mass balance conditions and solved for total concentration which are then compared to the analytical values (ref. 7). In the continued fraction method the non-linear equations are rearranged to solve for free ion concentrations which are initially assumed to be equal to the total concentrations.

Probabilistic and Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions are those that are inherent in the chemical equations such as the Debye-Huckel equation (see documentation).

Structure and Level of Detail - WATEQF is a general computer program for the calculation of chemical equilibria in natural waters at low temperatures. It may be expanded and updated by the user as additional stability data on complexes and minerals become available. An aqueous model model needs to be defined separately from the computer program which executes calculations based on the model. The choice of a model must be made on the basis of the problem to be solved and each model has its own set of assumptions and restrictions. A discussion of various chemical models can be found in Nordstrom et al. (ref. 7).

Major Dependent Variables - The principal variables of this program are:

- Debye-Hückel equation parameters and constants
- Stoichiometric coefficients
- Electrical imbalances of initial solutions
- Charge difference between the sum of anions and the sum of the cations

- Activity product and saturation state

- Total concentration of elements in solution

Applicability, Limitations, Validity, and Completeness - WATEQF is a general chemical equilibria program suited for low temperature natural waters. Several conceptual and numerical limitations should be considered.

- There is no proton mass balance condition, only mass balances on cations and anions are considered.

- Uses the Van't Hoff equation or analytical expressions for equilibrium constant as a function of temperature and is only reliable for the range 0-100 °C.

- Lacks important minerals such as minerals of uranium but program can be updated.

- Reliability of the equilibrium constants is the most important factor in equilibrium programs. All models must be updated as needed.

- WATEQF should not be used in water whose salinity exceeds that of sea water.

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6.0 HEAT TRANSPORT CODES

6.1 CCC

Area: Repository Siting
Repository Design

I. Summary of Code

Purpose and Scope - CCC (Conduction-Convection-Consolidation) models heat and fluid flow in a two- or three-dimensional saturated porous medium and calculates the one-dimensional consolidation (subsidence) of the medium.

Authors - The program was developed by D.C. Mangold, M.J. Lippmann, and S.G. Bodvarsson at Lawrence Berkeley Laboratory.

Code Functions - The movement of heat and a single fluid phase are modeled. The mass-flow equation is time-dependent and takes account of sources, sinks, and specific storage. The energy equation takes account of conduction, convection, and sources and sinks. Porosity and specific storage vary with the effective stress on the rock; thermal conductivity, rock and fluid heat capacity, and fluid viscosity vary with temperature; permeability varies with both temperature and effective stress; and fluid density varies with temperature and pressure. The two equations are solved simultaneously using the integrated finite-difference method.

Potential Usage - CCC can be used in situations where subsidence might be significant to calculate water-flow fields. It can provide both the flow time to the accessible environment and the input to a solute transport code such as FEMWASTE, MMT, or NUTRAN.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 40, and 75.

Restrictions - None; the program is available from the Argonne Code Center.

II. Summary of Findings

General Critique - CCC is unique in that it solves for flow and heat transport in a liquid saturated medium, and computes one-dimensional consolidation. The appropriate equations are solved using the integrated finite-difference method.

The consolidation portion of the code is designed primarily for one-dimensional compression that results from decreasing the pore pressure as a result of pumpage. This will probably not be of particular importance in a high-level radioactive waste repository, given the probable presence of a thick overburden.

CCC is one of the principal codes used to examine thermal energy storage problems in aquifers.

Applicability to Medium - CCC should be applicable to any medium other than salt. Varying brine densities would make it inappropriate for salt. Also chemical changes not included in the code might make it difficult to apply it to shales.

Sensitivity Analysis - The code has had many sensitivity analyses, including testing of both physical and numerical parameters.

Code Verification - CCC has been tested against several analytical solutions and is considered well verified. The main concern is how often one-dimensional consolidation is a valid assumption.

Field Validation - This code has been applied to several field problems dealing with aquifer thermal energy storage, the problem for which the code was primarily designed (ref. 6).

III. General Description

Operating Characteristics - The code is written in FORTRAN IV.

Inputs - The principal inputs are as follows:

- Initial temperatures
- Initial fluid densities
- Initial pressures
- Mass injection rates
- Heat content of injected fluid at each injection point
- Density of each rock type
- Specific heat of each rock type as a function of temperature
- Thermal conductivity of liquid-solid mixture for each rock type as a function of temperature
- Intrinsic permeability of each rock type as a function of temperature
- Specific storage of each rock type
- Ratio of vertical to horizontal permeability in each rock type
- Ratio of vertical to horizontal thermal conductivity in each rock type
- Porosity of each rock type
- Coefficient of compressibility of each rock type
- Swelling index of each rock type
- Compression index of each rock type
- Dynamic viscosity as a function of temperature
- Fluid compressibility as a function of temperature
- Fluid specific heat as a function of temperature
- Fluid equation of state

Outputs - All the thermal and mass flows and other quantities which are stored can be printed out for each node. The degree of consolidation can also be output.

Available Documentation - A user's guide has been published (ref. 1).

IV. Review of Theory

Equations - The integrated finite-difference method (IFDM) does not require a rectangular grid. Though less commonly applied than the conventional finite-difference approach, the IFDM has been used to study ground-water problems since the early 1960's, when it was known as a polygonal model technique.

For the IFDM, the region of interest must be divided into smaller areas known as nodal areas, since they each have a node point which is used for mathematical purposes to connect each area with its neighbor. CCC divides the study region into polyhedrons by bisecting the lines connecting nodal points.

The two key equations are the mass balance:

$$\frac{(S_s V)_n}{g} \frac{\Delta P_n}{\Delta t} = \sum_m \left[\left(\frac{k\rho A}{\mu} \right)_{n,m} \frac{(P_m - P_n)}{D_{n,m}} - \left(\frac{k\rho^2 \eta A}{\mu} \right)_{n,m} g \right] + (G_f V)_n \tag{6.1}$$

and the energy balance:

$$(\rho c)_M V_n \frac{\Delta T_n}{\Delta t} = \sum_m \left[\frac{(K_M A)_{n,m}}{D_{n,m}} (T_m - T_n) + \left(\frac{\rho c_F A k}{\mu} \right)_{n,m} (T_{n,m} - T_n) \left(\frac{P_m - P_n}{D_{n,m}} - \eta \rho g \right) \right] + (G_h V)_n \tag{6.2}$$

where

- n and m refer to connected nodes
- S_s is the specific storage
- V is the cell volume
- g is the acceleration of gravity
- P is the water pressure
- Δ indicates the change over one time step
- t is time
- k is intrinsic permeability
- ρ is fluid density
- A is the area of the surface connecting two adjacent cells
- μ is dynamic viscosity
- D is the distance between two node points
- η is the direction cosine between the vertical and the vector from node n to node m
- G_f is the fluid source or sink
- K_M is the thermal conductivity of the rock-fluid mixture
- T is temperature
- c is fluid heat capacity
- G_n is the heat source or sink

$(\rho c)_M$ is given by

$$(\rho c)_M = \phi \rho_f c_f + (1 - \phi)\rho_s c_s \tag{6.3}$$

where ϕ is porosity and f and s refer to fluid and solid.

Deformation is calculated in one dimension by the Terzaghi theory. This is based on the relationship between P and the effective rock stress σ', which is defined as

$$\sigma' = \sigma_N - P \tag{6.4}$$

where σ_N is the overburden (normal stress). The void ratio e, defined by

$$e = \frac{\phi}{1-\phi} \tag{6.5}$$

is plotted against log σ'. These curves are approximated by straight lines, one of slope C_c for virgin loading, and others of slope C_s for unloading and loading below previously attained stresses.

The storage and permeability are computed from:

$$S_s = \rho g \left[\phi\beta + \frac{a_v}{1+e} \right] \tag{6.6}$$

$$a_v = \frac{C_c}{2.303\sigma'} \tag{6.7}$$

$$k = k_o \exp\left[\frac{2.303(e-e_o)}{C_k} \right] \tag{6.8}$$

where β is the fluid compressibility, k_o and e_o are arbitrary, and C_k is an empirical constant.

Numerical Approximations - The following are the key numerical approximations in CCC:

- Discretization of space and time
- Use of linear consolidation curves
- Linear interpolation of temperature dependence of material properties
- The heat and mass transfer equations are solved alternately, with overlapping time steps.

The basic equations are solved using the integrated finite-difference method. The basic idea is to solve the equations directly without reducing them to point equations. The volume is selected to be a multi-faceted sphere (a polygon in two dimensions) where the flux across each face is approximated using a finite-difference approximation of these first order terms. To evaluate volume boundary temperatures, upstream weighting is used.

As with other finite-difference methods, it is assumed that all recharge or withdrawal to and from the nodal area occurs at the node point and that water levels in the entire nodal area are the same as at the node point. For this reason, the polygon geometry as well as rectangular grids should be kept to a reasonable size to maintain accuracy. The triangles formed by connecting the node points have no interior angle greater than 90° since the polygon sides are perpendicular bisectors of the lines connecting the intersects. When rectangular nodes are used, the interconnects form rectangles. Departures of more than 5 to 8 degrees from the 90^{0} limit will result in significant computational errors which cannot be easily identified in the results.

The pressure and energy equations are solved alternatively by interlacing them in time. Since, in general, the pressure changes much more rapidly than the temperature, much smaller time steps are used in the flow cycles than in the energy cycles. The resulting solution technique is called mixed explicit-implicit iterative scheme. The matrix solution technique is similar to successive over-relaxation.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions, other than those listed under numerical approximations, are as follows:

- The medium is saturated.
- Darcy's law adequately describes fluid movement.
- The rock and the fluid are in thermal equilibrium at any given time.
- Energy changes due to the fluid compressibility, acceleration, and viscous dissipation can be neglected.
- The one-dimensional consolidation theory can adequately describe the vertical deformation of the medium; lateral stresses in the overburden can be ignored.
- Permeability can be taken from the empirical formula (Equation 6.8).

Structure and Level of Detail - The code allows an arbitrary set of nodes, in 1, 2, or 3 dimensions, including Cartesian, cylindrical or spherical coordinates. It allows for steady or transient flow, heat transport, and consolidation in heterogeneous and/or anisotropic media. Boundary conditions may either be specified value or specified flux.

Major Dependent Variables - The code's major variables are the fluid flows, pressures, rock stresses, temperature, and heat flows.

Applicability, Limitations, Validity, and Completeness - The code was designed for aquifer thermal energy storage problems. The features of CCC that relate to subsidence are probably not of importance to repository siting. Although the code has not been extensively applied to radioactive waste management, it has potential value in the analysis of the effects of heat on ground-water flow.

References -

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6.2 SHAFT79

Area: Repository Siting
Repository Design

I. Summary of Code

Purpose and Scope - SHAFT79 (Simultaneous Heat and Fluid Transport) models fluid flow and heat transport in porous media. Transient problems involving both liquid and vapor phases can be solved. The code was originally designed to simulate two-phase geothermal reservoirs.

Authors - SHAFT79 was developed by Karsten Pruess, Ron C. Schroeder, Paul A. Witherspoon, and J. Mike Zerzan at Lawrence Berkeley Laboratory.

Code Functions - SHAFT79 calculates fluid flow and heat transfer in three dimensions using an integrated finite-difference method. The fluid must have only a single component, but may have liquid and vapor phases. Porosity can vary with pressure and temperature.

Potential Usage - SHAFT79 could be used to calculate the fluid flow around a repository during the thermal phase. The calculated water velocities would be input to a solute transport code such as DPCT or NUTRAN.

SHAFT79 could also be used to determine whether a site satisfied a requirement of minimum water flow time to the accessible environment, if such a requirement were be imposed on flow fields as perturbed by the repository.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 40, and 75.

Restriction - None; the code is available from the Argonne Code Center.

II. Summary of Findings

General Critique - SHAFT79 was originally designed for simulating two-phase geothermal reservoirs. The numerical approximation is the integrated finite-difference method. This method allows a flexible geometric description.

Unlike the other codes in this section, SHAFT79 simulates two-phase flow. The formation of steam in the repository is unlikely, but will depend on the designed heat generation of the canisters. If steam formation is not important, then a single-phase heat transport code is more appropriate, since the inclusion of two-phase flow increases the numerical difficulties and computer run times substantially. However, if steam does form, a code like SHAFT79 will be necessary to accurately account for the changes in the flow field.

An earlier version of this code, SHAFT, suffered from published results that contained errors in the thermodynamic properties. The code has since been rewritten and called SHAFT79. We are not aware of any similar problems with SHAFT79.

Applicability to Medium - SHAFT79 should be applicable to any medium other than salt. Varying brine densities would make it inappropriate for salt. Also, chemical changes not included in the code might make it difficult to apply it to shales.

Sensitivity Analysis - Some field geothermal problems have been analyzed for a variety of injection and pumping schemes. Also, some sample problems have been solved with more than one value of permeability and porosity.

Code Verification - Results of the code have been compared with a number of analytic and numerical solutions. This includes a set of problems provided in a DOE sponsored code comparison. Agreement has been excellent (usually within one percent of the analytic solutions).

Field Validation - The code was used to simulate the behavior of the Serrazzono geothermal field in Italy (ref. 4). The computed pressure decline was slower than observed by a factor of 3.5. This may be due to assumption of erroneous initial conditions rather than any shortcomings of the code itself. It has also been used in the early phases of geothermal reservoir development at the Baca Location, New Mexico (ref. 6).

III. General Description

Operating Characteristics - SHAFT79 operates on a CDC 7600 computer. It is written in FORTRAN IV. Because it used the integrated finite-difference method, it has similar restrictions to those described for CCC.

Inputs - The principal inputs to SHAFT79 are as follows:

Density of each type of rock
Porosity of each element
Permeability of each rock type along each principal axis
Thermal conductivity of each rock type
Specific heat of each rock type
Compressibility of each rock type
Coefficient of thermal expansion of each rock type
Initial fluid density in each element
Initial fluid internal energy in each element
Heat and mass output of thermal or fluid sources and sinks
Location of sources and sinks

Output - The principal outputs are:

(1) The production of heat flow, fluid flow, gas flow, or liquid flow, either cumulatively or per unit time.

(2) Values of various parameters in each element at selected time steps.

Available Documentation - A moderately complete user's manual has been issued (ref. 1).

IV Review of Theory

Equations - SHAFT79 treats two-phase systems in which the fluid can be either liquid or vapor. It solves the following discretized mass and energy balance equations:

$$\phi_n^{i+1}\rho_n^{i+1} - \phi_n^i\rho_n^i - \frac{\Delta t}{V_n}\left\{\sum_m F_{nm}^{i+1} + V_n q_n^{i+1}\right\} = 0 \qquad (6.9)$$

$$\phi_n^{i+1}\rho_n^{i+1}u_n^{i+1} - \phi_n^i\rho_n^i u_n^i + \left[(1-\phi_n)\rho_R\right]C_R\,(T_n^{i+1} - T_n^i) - \frac{\Delta t}{V_n}\left\{\sum_m G_{nm}^{i+1} + V_n Q_n^{i+1}\right\} = 0 \qquad (6.10)$$

Here, n, m label the volume elements, and i labels the time step. ϕ is porosity (void fraction), ρ is fluid density, q is a source term for mass generation, u is the specific internal energy of the fluid, G is energy flux, Q is an energy source term, ρ_R is the rock density, C_R is the specific heat of the rock, Δt is the duration of the time step, V is volume of the element, and T is temperature.

The mass flow F_{mn} from element m to element n is given by:

$$F_{nm} = A_{nm}\sum_\alpha k_{(nm)}\left(\frac{k_\alpha}{\mu_\alpha}\right)_{(nm)}(\rho_\alpha)_{(nm)}\left(\frac{P_m - P_n}{d_{nm}} - (\rho_\alpha)_{(nm)}g_{(nm)}\right) \qquad (6.11)$$

with interface area A_{nm} over a distance d_{nm}. Other terms include k and k_α, absolute and relative permeability, respectively, P, pressure, and g, gravitational acceleration. α has the values "liquid" and "vapor". An analogous definition holds for the energy flow G_{nm}. Whereas ϕ_n can vary with time, the apparent rock density $(1-\phi_n)\rho_R$ is constant. Different weighting procedures can be selected for the various "interface quantities," labeled with subscript (nm) (harmonic weighting, spatial interpolation, upstream weighting).

Numerical Approximations - The non-linear finite-difference equations are solved with the Newton/Raphson method. The set of linear equations arising at each iteration step is solved with an efficient direct solver, employing sparse storage techniques. The principal numerical approximations in SHAFT79 are the following:

- Discretization of time and space
- Use of an approximation to the steam tables.

As discussed, the space approximation is the integrated finite-difference method. Time is discretized using a first-order finite-difference approximation. This, along with the Newton-Raphson iteration, results in a fully-implicit solution.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions are the following:

- The physical systems described by SHAFT79 are approximated as systems of porous rock saturated with one-component fluid in liquid and vapor form.
- Except for porosity, which can vary with pressure and temperature, all other rock properties--density, specific heat, thermal conductivity, absolute permeability--are independent of temperature, pressure, or vapor saturation.
- Liquid, vapor, and rock matrix are in local thermodynamic equilibrium, i.e., at the same temperature and pressure, at all times.
- Capillary pressure is neglected.
- Relative permeability is described in the classical petroleum fashion.

Structure and Level of Detail - The code accommodates an arbitrary rectangular array of elements. The integrated finite-difference method allows for the approximation of fairly irregular geometries.

Major Dependent Variables - The key variables in the calculation are the pressures, rock and fluid temperatures, and flow vectors. Other important variables are listed in the section on equations. The code actually solves for fluid density and fluid specific internal energy.

Applicability, Limitations, Validity, and Completeness - For the problem for which the code was designed, it is fairly complete. If two-phase flow is important in a repository, however, it may be important to also consider the air phase. In addition, fluid pressure increases may cause fracturing. SHAFT79 does not consider problems of fracturing and does not consider the air phase.

References -

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6.3 MAGNUM2D

Area: Repository Siting
Repository Design

I. Summary of Code

Purpose and Scope - The MAGNUM2D model is designed to simulate ground-water flow and heat transport in fractured-porous rock systems.

Authors - MAGNUM2D was developed by Resource Management Associates, Lafayette, California, for the BWIP program.

Code Functions - The MAGNUM2D model is a two-dimensional finite-element code designed to simulate ground-water flow and heat transport in fractured-porous rock systems. The theoretical framework of the model is based on concepts for porous continua and for discrete conduits. A "dual porosity" approach is used to represent the continuous rock mass whereas flow through discrete channels are described in terms of Poiseuille flow in planar conduits.

The principal features of the MAGNUM2D code are as follows:

- Continuous rock mass represented with isoparametric finite elements; line elements are embedded along the sides of 2-D elements to represent discrete fractures.
- Model accommodates complex stratigraphic features with variable media properties.
- Computer code provides options for coupled or uncoupled solutions of heat and flow equations.

Potential Usage - MAGNUM2D can be used to calculate the fluid flow around a repository during the thermal phase. It provides flow field calculations for input to pathline and transport models. The difference between MAGNUM2D and the other heat transport codes discussed in this section is that it models fractured as well as porous media. Results from MAGNUM2D could provide boundary conditions to far-field flow codes, such as USGS2D or FE3DGW.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 35, 40, and 75.

Restrictions - MAGNUM2D is being used by the BWIP program at the Hanford site. The code is to be made available to the public, but documentation is not yet available.

II. Summary of Findings

General Critique - The code provides a two-dimensional simulation of fluid flow and energy transport through a fractured porous medium. Some of the assumptions regarding flow in fractured media are still at a research stage and have not been fully verified. The model couples the flow and heat transport equation.

These governing equations are solved using the finite-element Galerkin method. Two-dimensional isoparametric elements are used to discretize the porous matrix with one-dimensional elements to model the discrete fractures.

Due to the fact that the model is capable of analyzing a complex ground-water system, the use of the program would be very much restricted by the availability of data.

Applicability to Medium - The main application would be in the analysis of flow and transport in a fractured porous medium.

Sensitivity Analysis - An extensive sensitivity analysis of waste isolation in a basalt medium was performed using MAGNUM2D by Rockwell Hanford Operations (ref.1).

Code Verification - Three sample problems were used to test the ground-water flow and energy transport components of the MAGNUM2D model. The first compares MAGNUM2D's outputs to the analytical solution of a simplified flow problem. The second compares MAGNUM2D to analytical results for a thermal dispersion problem. The third examines MAGNUM2D's performance on a coupled heat and fluid flow (non-isothermal) problem which has been solved analytically. It should be noted that these comparisons were made using the code SEMTRA, the forerunner of MAGNUM2D.

Field Validation - Some work has been done at the Hanford site but it has been more of a hypothetical nature than a true field application.

III. General Description

Operating Characteristics - Since documentation is not yet available, this section cannot be completed.

Inputs - Inputs for MAGNUM2D include

Mesh geometry
Initial heads
Initial temperatures
Boundary conditions for both pressure and temperature
Heat transfer coefficient
Specific heat capacity of fluid
Hydraulic conductivity tensor
Density disparity factor
Heat source term
Specific storage coefficients
Coupling coefficient between primary and secondary pores
Thermal coupling coefficients
Heat dispersion tensor
Mass dispersion tensor
Primary and secondary porosities
Mass source term
Fluid density
Number of collocation points on the finite element.

Outputs - Output for MAGNUM2D consists of the hydraulic head and temperature in both the fractures and porous matrix at each time step.

Available Documentation - Documentation of MAGNUM2D is scheduled to be published during FY 1983.

IV. Review of Theory

Equations - The governing equations for the pressure distribution in the fractures and porous block of a fractured porous medium are given as:

$$\frac{\partial}{\partial x_i} K_{ij} \frac{\partial}{\partial x_j} (h + \delta_b x_3) = S_p \frac{\partial h}{\partial t} - \frac{I_s}{\rho} - \gamma_p \frac{\partial T}{\partial t} \qquad (6.12)$$

in the fractures and

$$0 = S_s \frac{\partial h_s}{\partial t} + \frac{I_s}{\rho} - \gamma_s \frac{\partial T}{\partial t} \qquad (6.13)$$

in the porous block, in which

$$I_s = \rho \beta_I (h_s - h)$$

$$\beta_I = 4K_m \phi_p / (c\ell)$$

$$\delta_b = (\rho - \rho_o)/\rho_o$$

$$\gamma_p = \rho_o \phi_p \beta_T / \rho \ (1/^oC)$$

$$\gamma_s = \phi_s \beta_T (1/^oC)$$

where:

S_p = specific storage for fractures (1/m)
g = acceleration of gravity (m/sec^2)
ρ_o = nominal density of water (kg/m^3)
ϕ_p = fracture porosity (dimensionless)
K_{ij} = fracture hydraulic conductivity tensor (m/sec)
x_3 = vertical elevation coordinate (m)
ρ = $\rho(T)$ = actual density of water at temperature T (kg/m^3)

K_m = scalar hydraulic conductivity for flow between fractures and pores (m/sec)
$c\ell$ = fracture shape factor (m^2)
β_T = coefficient of thermal expansion of water (1/°C)
S_s = specific storage for porous block (1/m)
T = temperature (°C)
ϕ_s = porosity associated with porous block (dimensionless)
h = hydraulic head in the fractures (m)
h_s = hydraulic head in the porous block (m)

The governing equation for the temperature distribution is given as:

$$\rho c\, K_{ij} \cdot \frac{\partial}{\partial x_j}(h + \delta_b x_3)\frac{\partial T}{\partial x_i} + \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial T}{\partial x_j}\right) = S_t \frac{\partial T}{\partial t} + Q \qquad (6.14)$$

where
S_t = $\rho c\, \phi_T + \rho_m c_m (1 - \phi_T)$ (Joule/m^3 °C)
c = specific heat of water (Joule/kg °C)
ρ_m = bulk density of the rock mass (kg/m^3)
c_m = specific heat of the rock mass (Joule/kg °C)
D_{ij} = thermal conductivity tensor (Joule/m °C sec)
ϕ_T = $\phi_p + \phi_s$
Q = thermal loading rate (Joule/m^3 sec).

Numerical Approximations - A finite-element solution technique applicable to the governing equations is developed by using the Galerkin method of weighted residuals. The dependent variables are approximated using quadratic shape functions. Temperature-dependent coefficients are fitted using spline functions. The finite-element equations are obtained by numerical integration over 2-D isoparametric elements and 1-D line elements.

Probabilistic or Statistical Aspects - In order to represent the fractured medium as a superposition of two continua with an exchange of mass between these continua, it is necessary to consider an REV (representative elementary volume) so as to obtain valid statistical averaging of the porosity and hydraulic conductivity of the fractured medium.

Assumptions and Simplifications - The principal simplifying assumptions are as follows:

- The fractured-porous medium is nondeformable.
- The fluid is slightly compressible.

- Macroscale (REV) hydraulic gradients are independent of fracture orientation or geometry.
- The fluid system is single-phase.
- The medium is fully saturated.
- Flow in fractures is governed by Darcy's equation.
- 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 in separately the primary and secondary storage systems, but conservation of energy applies in the system as a whole.

Structure and Level of Detail - The code is based on representing the flow and temperature fields using quadratic shape functions. The finite-element Galerkin method is used and the final equations are evaluated by numerical integration over 2-D isoparametric elements and 1-D line elements.

Major Dependent Variables - Aside from the input parameters the major variables are the hydraulic heads in the fractures and porous blocks and the temperatures.

Applicability, Limitations, Validity and Completeness - This model is able to perform a two-dimensional simulation of flow and energy transport through a fractured porous medium.

The code would be applicable if the fractures may be averaged over a representative volume. In this case, the fractures are approximated by a continuum. Alternatively, the fractures may be treated as being discrete. In this case the geometry of each fracture must be known.

References -

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7.0 SOLUTE AND HEAT TRANSPORT CODES

7.1 SHALT

Area: Repository Siting
Repository Design

I. Summary of Code

Purpose and Scope - SHALT (Solute, Heat, and Liquid Transport) was developed to simulate liquid flow, heat transport, and solute transport in a regional ground-water flow system.

Authors - SHALT was developed by J.F. Pickens and G.E. Grisak of the Inland Waters Directorate, Environment Canada for Atomic Energy of Canada, Ltd.

Code Functions - SHALT performs a two-dimensional finite-element simulation of fluid flow, energy and solute transport in an aquifer system. The aquifer to be modeled may be described in areal or cross-sectional coordinates. 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.

Potential Usage - 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.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 28, 40, and 75.

Restrictions - The code is public and is therefore available to the NRC.

II. Summary of Findings

General Critique - The code may be useful for the simulation of flow, energy and solute transport in a saturated ground-water system. Six types of boundary conditions are available consisting of specified flux or specified value of pressure, temperature and concentration. The model analyzes flow and transport in an aquifer from a plane cross-sectional or areal viewpoint.

SHALT is based on the finite-element method utilizing the Galerkin technique. The model is suitable for simulating the transport of liquid, heat, and solutes in a vertical-cross section coincident with the principal direction of flow in a ground-water flow system. A number of the system parameters are represented as functions of one or a combination of pressure, temperature, and concentration. Material properties of the porous medium may vary spatially. Stress/strain-permeability relationships that may exist have been neglected.

The three governing equations are solved sequentially with the temperature- or concentration-dependent variables updated after each time step. There is no iteration between time steps; this may induce errors if the time steps used are too large.

Three-noded triangular finite elements are used which have a distinct advantage over the finite-difference method when modeling boundary conditions having a complex boundary shape. Upstream weighting is not used; this may lead to numerical instability at early times for convection-dominated transport.

A significant disadvantage is that the code is not fully documented.

Applicability to Medium - The code is applicable to most porous media as long as vertical or horizontal averaging is valid and a two-dimensional simulation may be performed.

Sensitivity Analysis - None.

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 heat 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.

Field Validation - SHALT was used successfully to model results of pressure testing in fractured rock at Chalk River (ref. 4).

III. General Description

Operating Characteristics - SHALT is written in FORTRAN IV, but it is not known on which machine it is presently running. Detailed operating characteristics are unavailable.

Inputs - Inputs for 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
The bulk density

Outputs - The output of SHALT consists of the pressure, concentration and temperature distribution at each time step.

Available Documentation - Certain aspects of SHALT are well documented as "Finite Element Analysis of Liquid Flow, Heat Transport and Solute Transport in a Ground-Water Flow System: 1. Governing Equations and Model Formulation", by J.F. Pickens and G.E. Grisak (ref. 1). Full documentation is not available.

IV. Review of Theory

Equations - The liquid-flow equation describing the transient pressure distribution in the liquid phase in a saturated porous medium can be written in two dimensions as:

$$L(p) = \rho(\alpha + \beta\phi)\frac{\partial p}{\partial t}$$

$$= -\frac{\partial}{\partial x_i}\left\{\frac{\rho}{\mu}\left(k_{ij}\left(\frac{\partial p}{\partial x_j} + \delta_{2j}\,\rho g\right)\right)\right\} + Q^p = 0 \qquad (7.1)$$

where L is the differential operator defined in the flow region, p is the pressure, ρ is the density of the liquid phase, α is the vertical compressibility of the porous medium, ϕ is the porosity, β is the compressibility coefficient of the liquid phase, t is time, μ is the dynamic viscosity of the liquid phase, k_{ij} is the local intrinsic permeability tensor, δ is the Kronecker delta, g is the gravitational constant, and Q^p is the time rate of supply (positive) or extraction (negative) of liquid mass per unit volume. A thermal expansivity term has been omitted in Equation (7.1) since it can be shown to be small compared with the compressibility terms, $\rho(\alpha + \phi\beta)\frac{\partial p}{\partial t}$. It is assumed that β is a constant; k, α, ϕ and Q^p can vary spatially; and ρ and μ can vary spatially and are dependent on the temperature distribution.

The Darcy velocity $\vec{q}$ of the liquid phase is given as:

$$q_i = -\frac{1}{\mu\phi}\left[k_{ij}\left(\frac{\partial p}{\partial x_j} + \delta_{2j}\,\rho g\right)\right] \qquad (7.2)$$

where δ is the Kronecker delta.

The initial conditions necessary for the solution of Equation (7.1) are:

$$p(x_1,x_2,0) = \tilde{p}_o(x_1,x_2) \tag{7.3}$$

where $\tilde{p}_o$ are initial prescribed pressures and x_1 and x_2 are the Cartesian directions with x_2 the vertical.

The Dirichlet boundary conditions can be expressed as:

$$p(x_i,t) = \tilde{p}(x_i,t) \qquad \text{on } B_1 \tag{7.4}$$

and the Neumann boundary conditions can be expressed as:

$$\left\{\frac{1}{\mu}\left(k_{ij}\left(\frac{\partial p}{\partial x_j} + \delta_{2j}\,\rho g\right)\right)\right\} \bar{n}_i = -q_n^p \qquad \text{on } B_2 \tag{7.5}$$

Where $\tilde{p}$ are prescribed pressures, $B_1 + B_2 = B$, the total boundary of the region, q_n^p is the prescribed liquid flux across a Neumann boundary and $\bar{n}_i$ is the unit outward normal vector to the boundary.

The heat transport equation describing the transient temperature distribution of a fluid in a saturated porous medium can be written as:

$$L(T) = \left(\rho\phi C_{vw} + (1-\phi)\,\rho_s C_{vs}\right)\frac{\partial T}{\partial t} - \frac{\partial}{\partial x_i}\left[\bar{K}_{ij}\frac{\partial T}{\partial x_i}\right]$$

$$+ \rho C_{vw}\left(q_i \frac{\partial T}{\partial x_i}\right) + Q^w + Q^s = 0 \tag{7.6}$$

$$\text{where } \bar{K}_{ij} = \phi K_{ij}^w + (1-\phi)\,K_{ij}^s \tag{7.7}$$

and T is the temperature, C_{vw} is the heat capacity of the liquid phase at constant volume per unit mass, ρ_s is the density of the solid phase, C_{vs} is the heat capacity of the solid phase at constant volume per unit mass, K_{ij}^w is the thermal dispersion tensor for the liquid (which includes the effects of mechanical dispersion and thermal conduction), K_{ij}^s is the thermal conductivity tensor of the solid phase and Q^w and Q^s are liquid and solid point heat source or sink functions. This form of the equation includes dispersion (both conduction in liquid and solid phases and mechanical dispersion in the liquid phase), advection (both free and forced convection) and a heat source or sink. For the

parameters not already introduced in the liquid flow equation, it is assumed that C_{vw} is a constant and ρ_s, C_{vs}, K^w, K^s, q_x, q_z, Q^w and Q^s can vary spatially. The liquid heat source or sink function Q^w is related to the liquid source or sink function Q^p.

The initial conditions necessary for the solution of Equation (7.6) are:

$$T(x_i,0) = \tilde{T}_o(x_i) \tag{7.8}$$

where $\tilde{T}_o$ are the initial prescribed temperatures.

The Dirichlet boundary condition can be expressed as:

$$T(x_i,t) = \tilde{T}(x_i,t) \qquad \text{on } B_3 \tag{7.9}$$

and the Neumann boundary condition can be expressed as:

$$\left\{\left[\delta_{ij}\,\bar{K}_{ij} + \phi(1 - \delta_{ij})\,K^w_{ij}\right]\frac{\partial T}{\partial x_j}\right\}\bar{n}_i = -q_n^T \qquad \text{on } B_4 \tag{7.10}$$

where $\tilde{T}$ are prescribed temperatures, $B_3 + B_4 = B$, and q_n^T is the prescribed heat flux across a Neumann boundary.

The solute transport equation describing the transient concentration distribution of a dissolved constituent being transported in a saturated porous medium can be written

$$L(C) = -\frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - q_i\frac{\partial C}{\partial x_i} + (\phi + \rho_b K_d)\left(\frac{\partial C}{\partial t} + \lambda C\right) + Q^c = 0 \tag{7.11}$$

where ρ_b is the bulk density of the medium, K_d is the distribution coefficient, C is the concentration of the constituent in the solution, D_{ij} is the hydrodynamic solute dispersion tensor, λ is the radioactive decay constant and Q^c is the mass rate per unit volume for addition or removal at a source or sink. This form of the equation includes the effects of dispersion, advection, reversible instantaneous sorption

described by a distribution coefficient, a first-order reaction such as radioactive decay, and a source or sink for the dissolved constituent. For the parameters not already introduced in the liquid flow and heat transport equations, it is assumed that λ is a constant and ρ_b, K_d, D and Q^C can vary spatially. It is also possible to represent nonlinear sorption relationships instead of the linear function given by the distribution coefficient.

The initial conditions necessary for the solution of Equation (7.11) are:

$$C(x_i,0) = \tilde{C}_o(x_i) \tag{7.12}$$

where $\tilde{C}_o$ are initial prescribed concentrations.

The Dirichlet boundary conditions can be expressed as:

$$C(x_i,t) = \tilde{C}(x_i,t) \tag{7.13}$$

and the Neumann boundary conditions can be expressed as:

$$(\phi D_{ij}) \frac{\partial C}{\partial x_j} \overline{n}_i = q_n^C \tag{7.14}$$

where q_n^C is the prescribed dispersive solute flux.

Numerical Approximations - The Galerkin technique is used to determine approximate solutions to Equations (7.1), (7.6) and (7.11) under the prescribed initial and boundary conditions. The cross-sectional representation of the flow system is divided into an equivalent system of subregions, which in this case are triangular elements. Trial solutions are chosen of the form:

$$p^n(x,z,t) = \sum_{i=1}^{n} p_i(t)N_i(x,z) \tag{7.15}$$

$$T^n(x,z,t) = \sum_{i=1}^{n} T_i(t)N_i(x,z) \tag{7.16}$$

and

$$C^n(x,z,t) = \sum_{i=1}^{n} C_i(t)N_i(x,z) \tag{7.17}$$

where $N_i(x,z)$ $(i=1,2,...n)$ is a particular set of nondimensional spatial functions known as shape functions which satisfy the boundary conditions and $p_i(t)$, $T_i(t)$ and $C_i(t)$ are undetermined time-dependent coefficients defined at the n nodal points of the discretized system.

The time-dependent nature of the governing equations can be accommodated by employing a finite-difference scheme to approximate the time derivatives. It has been found (ref. 1) that the backward difference scheme provides better results than a Crank-Nicholson central difference approach for the time derivative of the solute transport equation.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions are as follows:

- Darcy's law is valid
- the compressibility and heat capacity of the liquid phase are constant
- k, α, ϕ and Q^P 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
- the hydrodynamic dispersion tensor for the liquid phase includes the effects of mechanical dispersion and thermal conduction and is a function of velocity

Structure and Level of Detail - 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.

Major Dependent Variables - Aside from the input parameters, the major variables are the nodal values of (1) pressure head, (2) concentration, and (3) temperature.

Applicability, Limitations, Validity and Completeness - A significant limitation in the use of this model is the fact that a two-dimensional simulation only may be performed. However, in many cases of bedded formations, the two-dimensional model would prove to be adequate.

References -

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7.2 SWIFT

Area: Repository Siting
Repository Design

I. Summary of Code

Purpose and Scope - SWIFT (Sandia Waste Isolation Flow and Transport) is a general nuclide transport code to describe migration from the repository through the ground-water system. It is based on the finite-difference method, and not only solves for flow and solute transport, but also solves for heat transport.

Authors - SWIFT was developed by R.T. Dillon at Sandia Laboratories and by R.B. Lantz and S.B. Pahwa at Intera, Inc.

Code Functions - The code simulates the flow and transport of energy, solute and radionuclides in a geologic media. SWIFT is a 3-D finite-difference ground-water 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
- Heat transport
- Well bore
- Heterogeneous and/or anisotropic media
- Confined and/or water-table conditions
- Recharge and/or wells.

Potential Usage - The code is fairly general and can be used to examine most far-field problems. It contains many options in terms of geometry, processes, and boundary conditions. Because it contains heat flow, it may also be used to examine some near-field problems. A more recent version, not documented, considers flow in fractured media. This version is not yet generally available.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 28, 40, and 75.

Restrictions - The code is available to the NRC.

II. Summary of Findings

General Critique - The code may be useful for the fully three-dimensional simulation of ground-water flow, energy, solute and radionuclide transport in a saturated geohydrologic system. Due to the complexity of the four coupled governing equations, it is necessary for the solution of these equations to be performed in a sequential manner.

SWIFT is a multipurpose code and may solve many engineering problems involving combinations of flow and transport. The code, however, may be too comprehensive when required for use for relatively less complex engineering problems and put too great a burden on user understanding.

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. As a result, the internals of SWIFT are difficult to understand and code modification is very difficult. In addition, because of the various options, code use is also difficult.

Applicability to Medium - SWIFT is a general purpose code and is applicable to most geologic media. The main limitation would be due to the availability of data. It may be valid in many cases to perform a horizontal or vertical averaging. SWIFT may still be used to perform a one- or two-dimensional simulation for this purpose.

Sensitivity Analysis - Sensitivity analysis has been performed on both physical and numerical parameters.

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.

Field Validation - None. SWIP, the forerunner of SWIFT, has been successfully applied to several field problems (e.g., ref. 5) by the U.S. Geological Survey.

III. General Description

Operating Characteristics - SWIFT is written in FORTRAN IV for use on a CDC 6600 machine. With minor modification, it can be used on other machines. This modification primarily involves the real-time dimensioning feature of SWIFT.

Inputs - 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 fluid in each well
Thermal diffusivity of rock surrounding wellbores
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
Leaching time of wastes

Outputs - 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.

Available Documentation - SWIFT is thoroughly documented in Ref. 4.

IV. Review of Theory

Equations - The equations describing fluid flow, energy, solute and radionuclide transport are obtained by combining the appropriate continuity and constitutive relations. The resulting equations may be stated as follows:

1) The governing equation for the fluid flow

$$\frac{\partial}{\partial x_j}\left(\frac{\rho k_{ij}}{\mu}\frac{\partial}{\partial x_j}(p - \rho g z)\right) - q + Q' = \frac{\partial}{\partial t}(\phi\rho) \qquad (7.18)$$

where

ρ = fluid density
k_{ij} = permeability tensor
μ = fluid viscosity
z = depth below some reference datum
p = pressure
ϕ = porosity
q = rate of fluid withdrawal
Q' = rate of production of brine due to salt dissolution
g = acceleration of gravity

The velocity vector v_i may be obtained from Darcy's law as:

$$v_i = -\frac{k_{ij}}{\mu} \frac{\partial}{\partial x_j} (p - \rho g z) \tag{7.19}$$

2) The governing equation for the energy transport

$$\frac{\partial}{\partial x_i} \left(E_{ij} \frac{\partial T}{\partial x_j}\right) - \frac{\partial}{\partial x_i} (\rho H v_i) - q_L - qH - q_H = \frac{\partial}{\partial t} \left[\phi \rho U + (1-\phi)\rho_R c_{pR} T\right] \tag{7.20}$$

where

E_{ij} = thermal hydrodynamic dispersion tensor
T = temperature
H = fluid enthalpy
q_L = heat loss to under/overburden
qH = heat source
q_H = rate of enthalpy removal
U = specific internal energy
ρ_R = formation density
c_{pR} = specific heat of the rock.

3) The governing equation for the solute transport

$$\frac{\partial}{\partial x_i} \left(\rho D_{ij} \frac{\partial}{\partial x} \hat{C}\right) - \frac{\partial}{\partial x_i} (\rho \hat{C} v_i) - q\hat{C} - q_c + Q_s = \frac{\partial}{\partial t} (\phi \rho \hat{C}) \tag{7.21}$$

where

D_{ij} = hydrodynamic dispersion tensor
$\hat{C}$ = solute concentration
q_c = rate of dissolved salt withdrawal
Q_s = salt dissolution rate

4) The governing equation for radionuclide component r

$$\frac{\partial}{\partial x_i}\left(\rho D_{ij}\ \frac{\partial C_r}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\rho C_r v_i\right) - qC_r - q_{cr}$$

$$+ q_{or} + \sum_{s=1}^{N_s} \lambda_{sr} R_s \phi\rho C_s - \sum_{\ell=1}^{N_\ell} \lambda_{r\ell} R_r \phi\rho C_r$$

$$= \frac{\partial}{\partial t}\left(\phi\rho R_r C_r\right) \qquad (7.22)$$

where

q_{cr} = rate of radionuclide withdrawal
q_{or} = waste leach rate
N_s = number of species decaying into component r
N_ℓ = number of species generated from the decay of species r
C_r = concentration of species r
λ_{sr} = the decay constant of species s into species r
R_r = equilibrium adsorption constant for species r.

Several quantities in Equations (7.18) to (7.22) require further definitions in terms of the basic parameters. The dispersion tensors may be expanded as follows:

Hydrodynamic dispersion = mechanical dispersion + molecular diffusion

$$D_{ij} = D'_{ij} + D^*_{ij} \qquad (7.23)$$

Thermal Hydrodynamic dispersion tensor = mechanical dispersion + conduction

$$E_{ij} = \rho c_{pw} D'_{ij} + K^*_{ij} \qquad (7.24)$$

Porosity is defined as

$$\phi = \phi_o\left[1 + c_R\,(p-p_o)\right] \qquad (7.25)$$

Fluid density is defined as

$$\rho = \rho_o\left[1 + c_w\,(p-p_o) + c_T\,(T-T_o) + c_s\hat{C}\right] \qquad (7.26)$$

Fluid viscosity is defined as

$$\mu = \mu_R(\hat{C}) \exp\left[B(\hat{C})\ (T^{-1} - T_R^{-1})\right] \qquad (7.27)$$

The subscripts o and R denote reference values, B is a function, and the c's are constants, except for c_s which is defined in terms of an input density range $(\rho_I - \rho_N)$,

$$c_s = (\rho_I - \rho_N)/\rho_o \qquad (7.28)$$

Numerical Approximations - The governing equations of fluid flow, energy, solute and radionuclide transport are solved by dividing the region of interest into a three-dimensional grid and developing finite-difference approximations for this grid. Once the region of interest is divided into grid blocks, finite-difference equations are developed whose solution closely approximate the solution of Equations (7.18) to (7.22). The resulting matrix equation is solved by different options, including L2SOR iterative and direct ordered Gaussian elimination.

Probabilistic or Statistical Aspects - None. The code is too complex to run many times for statistical purposes.

Assumptions and Simplifications - The principal simplifying assumptions (other than those listed under numerical approximations) are as follows:

- 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.
- Injected wastes are miscible with the inplace 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 equations 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.

Structure and Level of Detail - 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. Because of the complex nature of the code, it has a very high level of detail in representing the various processes.

Major Dependent Variables - Aside from the input parameters, the major variables are the pressures, the temperatures, solute concentrations and the concentration of each radionuclide species.

Applicability, Limitations, Validity and Completeness - Due to its generality, SWIFT has many applications. They include, but are not limited to, the following:

- nuclear waste isolation in various geologic formations
- injection of industrial wastes into saline aquifers
- heat storage in aquifers
- in situ solution mining
- migration of contaminants from landfills
- disposal of municipal wastes
- salt-water intrusion in coastal regions
- brine disposal from petroleum-storage facilities
- determination of aquifer transport parameters from well test data.

The principal limitation of the code is its complexity and difficulty of use. Also node spacing and time steps are limited to maximum values. This might make simulation of large-scale, long-period problems difficult.

References -

1. Dillon, R.T., R.B. Lantz, and S.B. Pahwa, "Risk methodology for geologic disposal of radioactive waste: The Sandia waste isolation flow and transport (SWIFT) model," Sandia National Laboratories Report SAND 78-1267, 1978.

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8.0 SOLUTE TRANSPORT CODES

8.1 CHAINT Area: Repository Siting

I. Summary of Code

Purpose and Scope - The CHAINT model is designed to simulate the transport of radionuclides in a fractured porous medium.

Authors - CHAINT was developed by Resource Management Associates, Lafayette, California for Rockwell Hanford Operations.

Code Functions - 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 2-dimensional elements.

Potential Usage - The code can be used to compute the concentrations of radionuclides entering the accessible environment. These results can be used as input to a dose calculation. Principal input to the code is the ground-water flow calculation obtained with the MAGNUM2D code (or a comparable nonisothermal flow model).

Related NRC Issues (See Table 1-4) - 3, 7, 8, 40, and 75.

Restrictions - CHAINT will be made available to the public, but documentation is not yet available.

II. Summary of Findings

General Critique - The code may be useful for the two-dimensional simulation for the transport of radionuclides through a fractured porous medium. The model requires a flow-field input obtained from the MAGNUM2D code (or a comparable nonisothermal flow model). Due to the fact that the model is capable of analyzing a complex ground- water system, the use of the program would be very much restricted by the availability of data.

One major assumption that is used in CHAINT is that radionuclide transport in the vicinity of the repository can be adequately described with the single-porosity formulation. This assumption is invalid if diffusion from the fractures into the rock matrix is important.

Major features of the computer code include:

- Model formulation is generalized to handle any combination of nuclides (actinides, fission or activation products) with contrasting half-lives.

- Computational algorithm accommodates subzone calculations in which the region of active nodes, within the finite-element mesh, is varied with time as the problem progresses.

- Numerical algorithms are second-order correct and fully implicit.

Applicability to Medium - The radionuclide transport model would be applicable in a geohydrologic medium if a two-dimensional averaging is valid, either in a horizontal or vertical plane.

The main application would be in the use of analysis of radionuclide transport in a fractured porous medium, although the usage is restricted by the amount of data available.

Sensitivity Analysis - An extensive parametric and sensitivity analysis of radioactive waste isolation in a basalt medium was performed using CHAINT by Rockwell Hanford Operations (ref. 1).

Code Verification - The code CHAINT was tested against an analytical solution based on the uranium decay series.

Field Validation - None.

III. General Description

Operating Characteristics - Because documentation is forthcoming, the operating characteristics are unknown.

Inputs - Inputs for CHAINT are not clearly specified in the available documentation. They seem to include:

Mesh geometry
Half lives of the radionuclide contaminants
Retardation factor of each contaminant
Velocity field
Mass dispersion tensor
Nuclide splitting fractions
Decay constants
Secondary porosity
Mass source term
Fluid density
Initial parent concentrations
Initial daughter product concentrations

Outputs - Output for CHAINT consists of the concentration of each radionuclide in the fractures at each time step.

Available Documentation - Formal documentation of CHAINT is to be ready in the near future.

IV. Review of Theory

Equations - The governing equation, based on the principles of conservation of mass, Fickian diffusion, and radionuclide decay, for the transport of radionuclides in a porous medium is described by the advection-diffusion equation:

$$\frac{\partial(\phi R_r C_r)}{\partial t} = -\frac{\partial}{\partial x_i}(C_r v_i) - \frac{\partial}{\partial x_i}(J_{ri}) + Q_r \qquad (8.1)$$

where C_r is the concentration in the dissolved phase of radionuclide constituent r, ϕ is porosity, v_i is the Darcy velocity obtained from a flow code such as MAGNUM2D, R_r is the retardation factor of component r, J_{ri} is the dispersive flux of constituent r and Q_r is the net production/removal of constituent r.

Since the dispersive flux J_{ri} is assumed to be Fickian, it may be related to the concentration gradient as follows:

$$J_{ri} = -D_{ij}\left[\phi \frac{\partial}{\partial x_j}(C_r)\right] \qquad (8.2)$$

where D_{ij} is the hydrodynamic dispersion tensor.

Dispersion effects consist of both velocity-dependent (mechanical dispersion) and velocity-independent (molecular diffusion) processes.

The radionuclide decay component of CHAINT describes the source/sink term Q_r and is given by:

$$Q_r = m_r \sum_{s=1}^{N} \ell_{rs}\lambda_s R_s \phi C_s - \lambda_r R_r \phi C_r \qquad (8.3)$$

where m_r is the net external input/output rate of dissolved constituent r, ℓ_{rs} is the fraction of constituent s which decays to constituent r, λ_r is the decay constant of constituent r, N is the number of other constituents decaying to constituent r, R_s is the retardation factor for constituent s and C_s is the concentration of radionuclide component s.

Numerical Approximations - The finite-element solution uses the Galerkin method of weighted residuals. This method is based on forming the integral of the product of the residual error and a set of weighting functions, where the residual error is defined in terms of the specific partial differential equations and approximating functions for the dependent variables.

Probabilistic or Statistical Aspects - As part of the input to CHAINT, a flow field of the geohydrologic system is required. The flow code most compatible with CHAINT is the code MAGNUM2D. In order to represent the fractured medium as a superposition of two continua, a statistical average of the concentration of fractures per representative volume must be assumed. This assumption is made in MAGNUM2D.

Assumptions and Simplifications - The principal simplifying assumptions are as follows:

- The diffusive flux J_{ri} 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.

Structure and Level of Detail - The code is based on representing the flow and concentration field using quadratic shape functions. The finite-element Galerkin method is used and the final equations are evaluated by numerical integration over 2-D isoparametric elements and 1-D line elements.

Major Dependent Variables - Aside from the input parameters, the major variables are the concentrations of each radioactive constituent.

Applicability, Limitations, Validity and Completeness - This model is able to perform a two-dimensional simulation of radionuclide transport through a fractured porous medium.

The code would be applicable if the fractures may be averaged over a representative volume, so that this volume can be considered as a continuum. Alternatively, the fractures may be treated as being discrete. In this case the geometry of each fracture must be known.

It appears that by combining the codes MAGNUM2D and CHAINT, flow is described in both the fractures and the porous blocks. However, transport is considered in only the fractures. If this is true, then this approach ignores matrix diffusion; that is, diffusion of radionuclides into the porous blocks. This is a very important limitation because the diffusion into the porous blocks (rock matrix) can enhance the retardation by many orders of magnitude as compared to retardation by surface reactions in fissures only (ref. 3).

References -

1. King, I.P., D.B. McLaughlin, W.R. Norton, R.G. Baca, and R.C. Arnett, "Parametric and sensitivity analysis of waste isolation in a basalt medium," Rockwell Hanford Operations Report RHO-BWI-C-94, 1981.

2. Baca, R.G., R.C. Arnett, and I.P. King, "Numerical modeling of flow and transport in a fractured-porous rock system," Rockwell Hanford Operations Report RHO-BWI-SA-113, 1981.

3. Neretnieks, I., "Diffusion in the rock matrix: An important factor in radionuclide retardation?", Jour. Geophys. Res., Vol. 85, No. B8, p. 4379-4397, 1980.

8.2 MMT Area: Repository Siting

I. Summary of Code

Purpose and Scope - MMT (Multicomponent Mass Transport) calculates the transport of dissolved contaminants in ground water. It is available in two versions:

- A two-dimensional version which does not treat daughter nuclides formed by radioactive decay
- A one-dimensional version which does handle decay chains.

This summary will focus on the version that handles decay chains (MMT1D).

Authors - MMT was developed at Battelle Pacific Northwest Laboratories. The 2-D version was prepared by S.W. Ahlstrom, H.P. Foote, R.C. Arnett, C.R. Cole, and R.J. Serne. The work to include decay chains was done by J.F. Washburn, F.E. Kaszeta, C.S. Simmons, and C.R. Cole.

Code Functions - MMT calculates the transport of radionuclide chains along a one-dimensional path. Radionuclides may be present as more than one chemical species, and chemical reactions can be treated. It may be possible to vary the water velocity, retardation factor, dispersivity, etc., along the path. If this can be done, MMT could be used to simulate transport along a network of flow paths as long as there are no branches in the network.

Potential Usage - MMT should be used in conjunction with a water flow code (e.g., VTT) and a biosphere transport and dose code (e.g., PABLM) to calculate long-term effects of a repository. The 1-D version is applicable, speaking roughly, to the same sorts of situations as flow-network codes such as GETOUT or NWFT. Its unique advantage, as compared to these codes, is the ability to model nuclides which are present as more than one chemical species.

Related NRC Issues (See Table 1-4) - 3, 7, 8, and 40.

Restrictions - None. MMT has been released to the public.

II. Summary of Findings

General Critique - The principal advantages of the particle tracking method are its inherent stability and simplicity. The principal disadvantage is poor computational efficiency. The current versions of MMT have the additional disadvantage that decay chains can only be treated if the flow path can be represented by an unbranched series of one-dimensional path segments.

In most of the cases it can now handle, MMT would seem to have little to recommend it over more computationally efficient flow-network codes such as GETOUT, NUTRAN, or NWFT. The principal exception would be radionuclides which exist as several chemical species with differing velocities (as much experimental evidence concerning plutonium, for example, suggests); other flow-network codes cannot now handle this situation.

If decay chains were incorporated into a two- or three-dimensional version of MMT, it would have some advantages over finite-difference and finite-element codes in the areas of numerical accuracy and stability. We do not know whether this could be achieved without paying an excessive price in computing time.

MMT is written in FLECS, a higher order language which compiles into FORTRAN. This could cause severe problems in maintaining and modifying the code at any institution other than PNL.

Applicability to Medium - All media.

Sensitivity Analysis - The sensitivity of results to the number of particles used has been studied.

Code Verification - MMT was compared to analytic results from GETOUT for a variety of problems.

Field Validation - The 2-D version was compared to migration of tritium on the Hanford Reservation. Agreement was moderately good, with discrepancies consistent with data uncertainties.

Whether such studies constitute a real field validation of this or any other solute transport model is a controversial question. The solute transport models contain adjustable parameters (such as dispersivity) which cannot be independently measured. It can be argued that manipulation of these parameters would allow the models to simulate almost any observed data.

III. General Description

Operating Characteristics - The code runs in an interactive mode. It is written in FLECS, a high-order language which is compiled into FORTRAN IV, which in turn is compiled. Also, the portion of MMT which smoothes and reports the results is dependent on PNL I/O hardware. The code is now being converted to CDC equipment.

Inputs - The following are the principal inputs to MMT:

Initial inventory of each nuclide
Half-life of each nuclide
Distribution coefficient of each nuclide
Average water velocity
Dispersion constant
Pathway dimensions
Time leaching begins
Duration of leaching

Outputs - 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.

Available Documentation - A User's Guide (ref. 2) is available (PNL-3179). It is fairly complete.

IV. Review of Theory

Equations - The MMT code calculates the motion of a large number of discrete point particles. The position and weight of each particle vary over time.

The position of a particle at time t + 1 is given by

$$x_{t+1} = x_t + \frac{v}{B}\Delta t + \sqrt{24\alpha\frac{v}{B}\Delta t}\ R \qquad (8.4)$$

where v is the velocity, B the retardation factor, Δt the time step, α the dispersivity, and R a random number uniformly distributed between -0.5 and 0.5.

At each time step, the concentration of each species is calculated for a set of "cells" by summing the weight of the particles of that species in each cell and dividing by the volume of water in the cell. These concentrations may be used to calculate "source" and "sink" terms (typically due to chemical reactions). The weight of each particle in the cell is multiplied by a factor reflecting the "source" or "sink". In the case of simple radioactive decay, the weight ε is given by

$$\varepsilon_{t+1} = \varepsilon_t\, e^{-\lambda\Delta t} \qquad (8.5)$$

where λ is the decay constant of the species.

Radioactive decay chains are treated by creating new particles of daughter nuclides. The daughter particle is located by assuming that decay occurred at a random time during the time interval:

$$x^d_{t+1} = x^p_t + R^*\left[\frac{v}{B^p}\Delta t + \sqrt{24\alpha\frac{v}{B^p}\Delta t}\ R\right] + (1-R^*)\left[\frac{v}{B^d}\Delta t + \sqrt{24\alpha\frac{v}{B^d}\Delta t}\ R\right] \qquad (8.6)$$

Here the superscripts d and p refer to daughter and parent, R is again a random number between -0.5 and 0.5, and R* is a random number between 0 and 1. The weight of the daughter particle is calculated from the weight of the parent particle and the appropriate radioactive decay equation. One may choose to create one daughter particle in each time

interval for more than one parent particle. In this case x_t is the weighted-average position of the group of parent particles, and the weight of the daughter particle is adjusted appropriately.

The calculated discharge rates tend to include fluctuations due to the random element of particle motion. A number of methods can be used to smooth the outputs; the user can examine these interactively and choose the one that seems best.

Numerical Approximations - There are two key numerical approximations in MMT:

- Representation of the water flow by a one-dimensional path
- Representation of the contaminants by a relatively small number of discrete particles.

When chemical reactions are present, averaging concentrations over a cell introduces a further approximation. Other approximations include:

- Placing daughter particles at the center of a group of parents rather than randomly
- Allowing only one decay in a chain during a time step .

Probabilistic or Statistical Aspects - 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.

Assumptions and Simplifications - The principal assumptions, other than those listed above as numerical approximations, are as follows:

- The one-dimensional solute transport equation is valid
- Sorption may be represented by equilibrium adsorption.

Structure and Level of Detail - Fluid flow proceeds along a one-dimensional path. It may (this is not clear) be possible for the path to be non-uniform.

Major Dependent Variables - The major dependent variable is concentration.

Applicability, Limitations, Validity, and Completeness - MMT, in its one-dimensional version, is, for the most part, limited to simple unbranched 1-D flow paths which could be handled by other codes such as GETOUT or NWFT. Unlike these codes, it has the potential of treating nuclides which exist as more than one chemical species. However, if the code were applied to problems involving chemical reactions, numerical problems requiring considerable reprogramming might arise.

If decay chains were introduced into the 2-D version of MMT, it would have a much wider application. In this case the principal limitation of the code would be the relative computational inefficiency of particle-tracking methods. This problem is accentuated by MMT's requirement that daughter nuclides cannot decay in the time step during which they are created, which severely limits the code's use with short-half-life daughters.

References -

1. Ahlstrom, S.W., H.P. Foote, R.C. Arnett, C.R. Cole, and R.J. Serne, "Multicomponent mass transport model: theory and numerical implementation (discrete-parcel-random-walk version)," Pacific Northwest Laboratory Report BNWL-2127, May 1977.

2. Washburn, J.F., F.E. Kaszeta, C.S. Simmons, and C.R. Cole, "Multicomponent mass transport model: A model for simulating migration of radionuclides in ground water," Pacific Northwest Laboratory Report PNL-3179, July 1980.

8.3 NWFT/DVM Area: Repository Siting

I. Summary of Code

Purpose and Scope - NWFT/DVM (Network Flow and Transport/ Distributed Velocity Method) models fluid flow and transport of radionuclide chains. The rate at which nuclides enter ground water can be limited by both leach rates and equilibrium solubility. Water velocities can reflect density forces caused by non-uniformities in salt concentration.

Authors - 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 Distributed Velocity Method, developed by Campbell and Longsine of Sandia and Reeves of INTERA.

Code Functions - 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 ground water 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.

Potential Usage - NWFT/DVM is a far-field code. It is designed to analyze repositories in well stratified sedimentary rocks. Its greatest strength is in handling cases involving (1) decay chains involving moderate contrasts in half-life and retardation factor, which cause difficulties for analytic and Green's function codes, and (2) path lengths much greater than the dispersivity, which are difficult to analyze with finite-element and finite-difference methods. NWFT/DVM is intended for use as a complement to SWIFT or some other finite-difference or finite-element code; each of these codes would be most accurate when the other is weakest.

Related NRC Issues (See Table 1-4) - 3, 7, 8, and 40.

Restrictions - The code is available to the NRC and has been released to the public.

II. Summary of Findings

General Critique - NWFT/DVM is well suited for its intended task of complementing a finite-element or finite-difference model. Its useful features include calculation of the combined effects of leaching and equilibrium solubility, treatment of cases with path length much greater than the dispersivity, consideration of flows driven by brine density, and accurate handling of decay chains with moderate contrasts in half-life and retardation.

The principal limitation of the code is its use of a fixed path network corresponding to a well stratified sedimentary setting with two aquifers. This limitation is not inherent in the DVM method.

The computational efficiency of NWFT/DVM appears to be intermediate between finite-element or finite-difference codes and semi-analytic models such as GETOUT or NUTRAN.

Compared to a finite-difference or finite-element code (such as SWIFT or FE3DGW) or a particle tracking code (such as MMT), its main advantages lie in computational efficiency, treatment of long paths, and treatment of decay chains. Its primary disadvantage is the difficulty of handling inherently 3-D problems with a flow network. Numerical dispersion considerations will sometimes favor an finite-element or finite-difference code and sometimes favor the DVM method.

Compared to a code which uses a network of flow paths with Green's functions (NUTRAN) the principal advantages of NWFT/DVM lie in its treatment of decay chains and its consideration of brine density. Its principal disadvantages are the inflexibility of the flow network, numerical dispersion, and, probably, lesser computational efficiency.

Applicability to Medium - NWFT/DVM is designed for bedded media. The brine density feature would be particularly useful with bedded salt.

Sensitivity Analysis - The sensitivity of numerical dispersion to relevant input parameters has been carefully evaluated.

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.

Field Validation - None.

III. General Description

Operating Characteristics - The code is written in some version of FORTRAN. No further information is given in the documentation. 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.

Inputs - NWFT/DVM can read single or multiple data sets. If multiple data sets are read, identical inputs need not be repeated. The principal inputs are as follows:

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 begins
Cutoff time

Outputs - 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.

Available Documentation - Documentation for NWFT/DVM is currently being released. Sandia National Laboratories are preparing for the NRC a series of manuals that include (1) a user's guide (ref. 1), (2) lecture notes (ref. 2), and (3) problem set.

IV. Review of Theory

Equations - NWFT/DVM represents the flow field as a network of one-dimensional path segments. It calculates fluid flow and transport through the network. Fluid flow is calculated by simultaneously solving for all legs the equations:

$$q_{ji} = \frac{1}{R_{ij}} (P_i - P_j) + \rho_{ij} (D_i - D_j) \tag{8.7}$$

and

$$\sum_{i \neq j} q_{ji} = 0 \tag{8.8}$$

where q_{ji} is the flow along the path from node i to node j, P and D are the pressure and elevation at each node, ρ_{ij} is the average fluid density in the path segment, and R_{ij} is a "hydraulic resistance" given by

$$R = \frac{\mu L}{kA} \tag{8.9}$$

where μ is the viscosity of the fluid in the path segment, L is the path length, k is the permeability, and A is the cross-sectional area. Water density and viscosity are functions of brine density.

Transport can be handled in two ways: analytically or by the DVM method. Analytical transport is limited to chains of three or fewer nuclides having the same retardation factor. Solubility limits are not considered. The equations used are:

$$N_1(t) = \frac{N_1(0)}{2\tau} e^{-\lambda_1 t}[U(t)-U(t-\tau)H(t-\tau)] \tag{8.10}$$

$$N_2(t) = \left[\frac{N_2(0)\, e^{-\lambda_2 t}}{2\tau} + \frac{N_1(0)}{2\tau}\left(\frac{\lambda_1}{\lambda_2 - \lambda_1}\right)\left(e^{-\lambda_1 t} - e^{-\lambda_2 t}\right)\right] \cdot$$

$$\left[[U(t) - U(t-\tau)H(t-\tau)]\right] \tag{8.11}$$

$$N_3(t) = \left[\frac{N_3(0)}{2\tau} e^{-\lambda_3 t} + \frac{N_2(0)}{2\tau}\left(\frac{\lambda_2}{\lambda_3 - \lambda_2}\right)\left(e^{-\lambda_2 t} - e^{-\lambda_3 t}\right) + \right.$$

$$\frac{N_1(0)}{2\tau}\lambda_1\lambda_2\left(\frac{e^{-\lambda_1 t}}{(\lambda_2 - \lambda_1)(\lambda_3 - \lambda_1)} + \frac{e^{-\lambda_2 t}}{(\lambda_1 - \lambda_2)(\lambda_3 - \lambda_2)} + \right.$$

$$\left.\left.\frac{e^{-\lambda_3 t}}{(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3)}\right)\right] \cdot \left[[U(t) - U(t-\tau)H(t-\tau)\right] \tag{8.12}$$

where

t = time
$N_r(0)$ = inventory of isotope r at time t = 0
λ_r = decay constant of isotope r
τ = leach time
$H(x) = 0 \qquad x < 0$
$H(x) = 1 \qquad x \geq 0$

$$U(t) \propto \operatorname{erfc}\left(\frac{L_p - \bar{v}t}{\sqrt{4\alpha t\bar{v}}}\right) + e^{\frac{L_p}{\alpha}} \operatorname{erfc}\left(\frac{L_p + \bar{v}t}{\sqrt{4\alpha t\bar{v}}}\right) \tag{8.13}$$

where

α = dispersivity
$\bar{v}$ = average isotope velocity (accounting for retardation)
L_p = distance from source to discharge point

The distributed velocity method (DVM) is based on dividing the path into cells. Dispersion is treated by dividing the contaminant in each cell into packets with different velocities. The velocities, of which there are N, are chosen so as to divide a Gaussian distribution of velocities into intervals of equal area. For a single species, the amount $\rho(i,t)$ of the species arriving in cell i at time step t is given by

$$\rho(i,t) = \frac{D}{N} \sum_j \left[M_j\, \rho(i-k_j, t-1) + (1-M_j)\, \rho(i-k_j-1, t-1)\right] \tag{8.14}$$

In this equation, D represents radioactive decay:

$$D = e^{-\lambda \Delta t} \tag{8.15}$$

where λ is the decay constant and Δt is the time step. k_j is the number of entire cells which can be traversed in one time step at velocity V_j:

$$k_j = \left\| \frac{V_j \Delta t}{\Delta x} \right\| \tag{8.16}$$

The double bars indicate the integral part.

M_j is the fraction of cell i-k_j which lies a distance $V_j\Delta t$ from points within cell i:

$$M_j = k_j + 1 - \frac{V_j \Delta t}{\Delta x} \tag{8.17}$$

When a decay chain is involved, the creation of each species during the time interval by decay of its parents must be considered. The concentration of species r, ρ_r, is then given by

$$\rho_r(i,t) = \frac{1}{N} \sum_s D_{rs} \sum_j \left[M_j^{rs} \rho_s(i-k_j^{rs}, t-1) + (1-M_j^{rs}) \rho_s(i-k_j^{rs}-1, t-1) \right] \tag{8.18}$$

where s may be either r or any parent of r. When r=s, D, k_j, and M are calculated from Equations (8.15) - (8.17). When r≠s, D is the probability that an atom of species s at time t-1 will have decayed into species r by time t. This is taken from the Bateman equation. k_j^{rs} and M_j^{rs} are calculated by replacing V_j in Equations (8.16) and (8.17) with

$$V_j^{rs} = \frac{1}{\Delta t} \sum_{n=s}^{r} T_n V_j^n \tag{8.19}$$

where n indicates the species in the decay chain from s to r, T_n is the mean time spent as species n, and V_j is the velocity of the jth packet of species n. This neglects the additional dispersion due to the range of possible decay times.

The amount of species r entering solution during a time step is the lesser of $C_r q \Delta t$, where C_r is the solubility and q the water flow rate, or the inventory of species r which has leached but, as yet, has not dissolved. This latter inventory is the sum of the amount of species r which leaches in the current interval and the amount which leached in previous intervals but did not dissolve.

The size of time and space steps, Δt and Δx, can either be calculated by the program or input by the user. To avoid error, these quantities must satisfy several conditions discussed in ref. 1. It is not always possible to satisfy all these conditions simultaneously.

Numerical Approximations - The principal numerical approximations in NWFT/DVM are the following:

- Space and time are discretized

- A continuous velocity distribution is replaced by no more than seven discrete packets each with a single velocity
- Dispersion due to the occurrence of radioactive decay at different times within a single time step is neglected
- Pathway dimensions, permeability, porosity, and brine density are averaged along each path segment
- Viscosity and density are obtained from approximate functional representations
- Solubility calculations assume isotopic ratios are the same at all times.

Probabilistic or Statistical Aspects - The program itself has none. However, it includes a software interface which permits it to be run repetitively in a Monte Carlo mode, if random inputs are generated by another program.

Assumptions and Simplifications - The principal simplifying assumptions (other than those listed above under numerical approximations) are as follows:

- 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.
- Sorption can be represented as equilibrium adsorption.

Structure and Level of Detail - The code is based on representing the flow field as a network of one-dimensional path segments. The network of repository corridors would be represented as a single path segment. A borehole or shaft could also be represented by a path segment. The code is limited to a specific network of 15 path segments, corresponding to a repository in a bed with a simple stratigraphy.

Major Dependent Variables - The key variable in this code is the water velocity in each path segment. Other important variables are listed in the section on equations. The code solves for pressure and concentration.

Applicability, Limitations, Validity, and Completeness - The model seems to be applicable to many cases, including some not handled well by finite-element and finite-difference methods.

The principal limitation of the code is the restriction to a particular geometry of flow network. Extensive reprogramming would apparently be required to use it for sites without continuous strata and an aquifer above the repository. However, the DVM method should be applicable to many other situations for which the hydrology could be represented by a flow network. Some of the subroutines in NWFT/DVM would probably be usable in a more general DVM program.

The code also would not be applicable to near-field problems in which thermal effects are important.

References -

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

2. "NWFT/DVM lecture notes" (rough draft), Sandia National Laboratories.

3. Campbell, J.E., D.E. Longsine, and M. Reeves, "The distributed velocity method of solving the convective-dispersion equation," to be published.

8.4 GETOUT

Area: Repository Siting

I. Summary of Code

Purpose and Scope - GETOUT models the transport of radionuclide chains along a one-dimensional path.

Authors - 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 Burkholder, Cloninger, W.V. DeMier, and P.J. Liddell.

Code Functions - GETOUT uses analytical solutions of the solute transport equation for one-, two-, or three-member chains. Longer chains are approximated by using these solutions. Release may be either an impulse or band.

Potential Usage - GETOUT requires the results of a water flow calculation (by hand or by machine) as input. It writes output files which can be read by the biosphere transport and dose code PABLM (and potentially by other such codes) to compute doses.

It could be used to check compliance with EPA standards for total releases.

Related NRC Issues (See Table 1-4) - 3, 7, 8, and 40.

Restrictions - None; the code has been published.

II. Summary of Findings

General Critique - GETOUT is an excellent code to use for systems which can be modeled as a single one-dimensional transport path. Because of its widespread use in at least three countries, there is a high degree of confidence in its reliability.

Because past applications have been to cases with very little dispersion, some care should be taken to ensure that numerical problems are not present if GETOUT is used for problems involving moderate or high dispersion.

Applicability to Medium - Any medium, but only systems which can be described as one-dimensional flows.

Sensitivity Analysis - There has been extensive sensitivity analysis with the code, both at PNL and in Sweden (ref. 5).

Code Verification - Verification work by E.L.J. Rosinger at Whiteshell (ref. 4 and personal communication) uncovered problems in early unpublished versions of the code and confirmed the accuracy of the published version by comparison with analytic solutions.

Field Validation - None.

III. General Description

Operating Characteristics - GETOUT is written in FORTRAN IV and implemented on a UNIVAC-1100/44 EXEC-8 system. It is now being converted to CDC equipment.

Inputs - The principal inputs are as follows:

Time leaching begins
Duration of leaching
Path length
Pore velocity of water
Dispersion coefficient

Outputs - 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.

Available Documentation - A User's Guide has been published (ref. 1).

IV. Review of Theory

Equations - GETOUT uses analytical solutions to the solute transport equation for decay chains, which may be written

$$B_i \frac{\partial C_i}{\partial t} = D \frac{\partial^2 C_i}{\partial x^2} - V \frac{\partial C_i}{\partial x} - B_i \lambda_i C_i + B_{i-1} \lambda_{i-1} C_{i-1} \qquad (8.20)$$

where C is concentration, B is retardation factor, D is dispersion coefficient, V is pore velocity, and λ is the radioactive decay constant. The subscripts refer to position in the decay chain.

The equations are solved for an impulse release, for a decaying band release, and for a decaying step function release. The solutions are too complicated to display here, but are given in the paper by Burkholder and Rosinger (ref. 4). (The earlier reports on GETOUT present the solutions in an ambiguous form; the paper by Burkholder and Rosinger is the most reliable source.)

GETOUT uses explicit analytic solutions for chains with one, two, or three members. Longer chains are approximated by three-member chains.

Numerical Approximations - The principal numerical approximations in GETOUT are the following:

- Use of uniform one-dimensional flow path

- Chains of four or more nuclides are approximated by three-member chains

- Release of radioactivity into ground water in the form of an impulse or band

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifying assumptions (other than those listed above under numerical approximations) are as follows:

- Validity of the one-dimensional solute transport equation

- Sorption may be represented as equilibrium adsorption

- Infinite solubility of all elements

- Steady-state fluid flow

Structure and Level of Detail - Simple, uniform one-dimensional path.

Major Dependent Variables - The code solves for concentration.

Applicability, Limitations, Validity, and Completeness - GETOUT is applicable to problems with a uniform one-dimensional flow path. For such problems, it is highly appropriate.

References -

1. De Mier, W.V., M.O. Cloninger, H.C. Burkholder, and P.J. Liddell, "GETOUT - A computer program for predicting radionuclide decay chain transport through geologic media," Pacific Northwest Laboratories Report PNL-2970, August 1979.

2. Burkholder, H.C., M.O. Cloninger, D.A. Baker, and G. Jansen, "Incentives for partitioning high-level qaste," Nuclear Technology, Vol. 31, p. 150, also as Pacific Northwest Laboratories Report BNWL-1927, 1976.

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

4. Burkholder H.C. and E.L.J. Rosinger, Nuclear Technology, Vol. 49, 1980.

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

8.5 DPCT Area: Repository Siting

I. Summary of Code

Purpose and Scope - DPCT (Deterministic-Probabilistic Contaminant Transport) simulates ground-water flow and contaminant transport in a two-dimensional cross-section. It can account for advection, dispersion, radioactive decay, and equilibrium sorption for a single contaminant.

Authors - DPCT was developed by Franklin Schwartz and A. Crowe of CGS, Inc.

Code Functions - 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 might be able to treat non-equilibrium sorption with a relatively minor modification.

Potential Usage - 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 two-dimensional cross-section can describe a wide variety of geologic settings. The principal limitation of the code is its inability to describe decay chains.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - None. The code has been published.

II. Summary of Findings

General Critique - DPCT is very similar in content to the two-dimensional version of MMT. However, it should be considerably easier than MMT to use, due to its better documentation, programming in a standard language, and better input formats. The two principal differences between the codes are that DPCT calculates water flow and their handling of chemical reactions.

If decay chains are not important, the choice between DPCT and a finite-element or finite-difference code would rest on a tradeoff between the stability and simplicity of the particle-tracking method and its lesser computational efficiency. It is not clear how much work would be required to incorporate decay chains in DPCT.

Compared with pipe-network codes, DPCT has advantages and disadvantages similar to those of FE and FD codes. Greater ability to treat inherently two-dimensional phenomena is counterbalanced by poorer computational efficiency and problems in representing small permeable features.

The manner in which sorption is treated by DPCT suggests that it might not be too difficult to modify the code to handle non-equilibrium ion exchange. If such a feature were developed, it would be quite unusual and possibly very useful.

Applicability to Medium - All media.

Sensitivity Analysis - Unknown; not described in user's guide.

Code Verification - Unknown; not described in user's guide.

Field Validation - Unknown; not described in user's guide.

III. General Description

Operating Characteristics - The program is written in FORTRAN IV and has been run on an Amdahl 470V/7 computer.

Inputs - The following are the principal inputs to DPCT:

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
Contaminant input rates and locations

Outputs - 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.

Available Documentation - An excellent user's manual is available (ref. 1).

IV. Review of Theory

Equations - The program first calculates the heads, h, by using finite elements to solve

$$\frac{\partial}{\partial x_i}\left(T_{ij}\,\frac{\partial h}{\partial x_j}\right) = 0 \qquad (8.21)$$

where T is the transmissivity tensor. Velocities are then determined by taking the gradient of h numerically.

In each time step, each particle takes steps which reflect both advective transport and dispersion. The new position $\overrightarrow{x_{t+1}}$ is given by

$$\vec{x}_{t+1} = \vec{x}_t + \vec{v}\Delta t + \sqrt{24\Delta t}\ A\ \vec{v} \tag{8.22}$$

$$A = \begin{pmatrix} \alpha_L R_L & \alpha_T R_T \\ \alpha_T R_T & \alpha_L R_L \end{pmatrix} \tag{8.23}$$

where Δt is the duration of the time step, $\vec{v}$ is the velocity, α_L and α_T are the longitudinal and transverse dispersion constants, and R_L and R_T are random numbers uniformly distributed between -0.5 and 0.5

Radioactive decay is accounted for by assigning each particle a weight ε. The weight is changed during each time step by

$$\varepsilon_{t+1} = \varepsilon_t\, e^{-\lambda\Delta t} \tag{8.24}$$

where λ is the radioactive decay coefficient.

Sorption is approximated as equilibrium cation exchange. The distribution coefficient K_d is calculated from the exchange capacity by

$$K_d = \frac{\sigma f'}{\beta} \tag{8.25}$$

where β is the total cation concentration in the solution and f' is a selectivity coefficient. Sorption is incorporated into the transport calculations by decreasing the weights of the particles; how this is done is not described.

Numerical Approximations - There are two key numerical approximations in DPCT:

- Water flow is calculated by finite elements at a set of discrete node points and interpolated linearly between them.
- The contaminants are represented by a relatively small number of discrete particles.

There is probably a further approximation in the treatment of sorption; the details of this are not well documented.

Probabilistic or Statistical Aspects - 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.

Assumptions and Simplifications - The principal assumptions, other than those listed above as numerical approximations, are as follows:

- 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.
- Ground-water flows are steady-state.

Structure and Level of Detail - The code represents a two-dimensional cross-section as a rectangular network of node points.

Major Dependent Variables - The code solves for hydraulic head and concentration.

Applicability, Limitations, Validity, and Completeness - The principal limitations on the use of the code are the absence of decay chains and the relative computational inefficiency of the particle-tracking method.

References -

1. Schwartz, F.W. and A. Crowe, "A deterministic-probabilistic model for contaminant transport," U.S. Nuclear Regulatory Commission Report NUREG/CR-1609, August 1980.

2. CGS, Inc., "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 1980.

3. Schwartz, F.W., "Application of probabilistic-deterministic modeling to problems of mass transport in groundwater system," Third International Hydrology Symposium, Ft. Collins, pp. 281-296, 1978.

Detailed derivations are given in:

4. Ahlstrom, S.W., H.P. Foote, R.C. Arnett, C.R. Cole and R.J. Serne, "Multicomponent mass transport model: theory and numerical implementation (discrete-parcel-random walk version)," Battelle Pacific Northwest Laboratory Report PNL-2127, 1977.

8.6 NUTRAN

Area: Repository Siting (with some Repository Design and Waste Package)

I. Summary of Code

Purpose and Scope - NUTRAN calculates the consequences (in terms of releases of radioactivity or doses to humans) of ground-water 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).

Authors - 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 Functions - 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 ground water 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 ground water through wells
- Transport of waste in surface waters and associated ecosystems
- Human exposure and dose mechanisms.

Potential Usage - NUTRAN performs most of the functions involved in analyzing long-term effects of a waste repository. NUTRAN contains only an extremely simple model for ground-water 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.

Related NRC Issues (See Table 1-4) - 3, 7, 8, and 40.

Restrictions - TASC has not released the program to the public. However, the code was developed with NRC funding and should be available to NRC.

II. Summary of Findings

General Critique - NUTRAN is a flexible and relatively efficient code applicable to many repository analyses. Its strengths include its incorporation of fairly simple models of several phenomena and the wide range of situations in which it can be used. A particular strength is in dealing with problems in which both natural and engineered barriers are present.

NUTRAN shares the strengths and weaknesses of other flow-path-network codes, such as NWFT/DVM and MMT. Among the strengths are computational efficiency and ability to handle small permeable features. The principal disadvantage is difficulty in handling problems with smooth gradients in two or three dimensions.

One advantage of NUTRAN over NWFT/DVM and MMT is flexible structure made possible by use of the PL/I language which allows the user much freedom in specifying path networks without reprogramming. A disadvantage of NUTRAN may be its approximate treatment of decay chains.

NUTRAN can handle transient flows in a rather inefficient manner. It may not be able to solve some problems with complex flow changes. However, NUTRAN's method tends to be well suited to handle effects of sudden future geologic changes.

Applicability to Medium - In general, NUTRAN is applicable to any medium, but it is better suited to settings which are well stratified or in which most flow is through a few small openings.

Sensitivity Analysis - Results of extensive sensitivity analysis have been published (ref. 6).

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

Field Validation - None.

III. General Description

Operating Characteristics - 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.

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
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.

Outputs - 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.

Available Documentation - Program documentation has been released (ref. 7).

IV. Review of Theory

This review will deal with WASTE and PLOT, excluding ORIGEN and the surface transport code BIODOSE.

Equations - WASTE treats the movement of a normalized concentration c of each radionuclide, defined by

$$c = \frac{C}{I} \tag{8.26}$$

where C is the concentration and I is the total inventory of the nuclide.

Radioactivity begins to leave the repository storage rooms at a time T_{rel} given by

$$T_{rel} = T_{cool} + \max [T_{fill}, T_{pen}] \tag{8.27}$$

where T_{cool} is the age of the waste at emplacement and T_{pen} is the canister lifetime. The repository resaturation time T_{fill} is either input or calculated from

$$T_{fill} = \frac{a}{Q_s} \frac{Men + 2DS_s(H_a+H_s)}{\frac{H_a}{|H_s|} + \frac{H_b}{H_b-H_a-H_s}} \tag{8.28}$$

where

Q_s is the steady-state inflow to the repository after resaturation is complete
a is the area of the mine
M is the height of rooms
e is the extraction ratio
n is the porosity of backfill
D is the distance to the aquifer
S_s is the specific storage of the rock mass
H_a is the height from the repository to the piezometric level of the overlying aquifer
H_b is the height from the repository to the piezometric level of the underlying aquifer
H_s is the head difference between the repository and the overlying aquifer in the post-resaturation steady state.

Beginning at T_{rel}, the waste matrix leaches at either a constant rate, a rate proportional to the remaining amount of waste, or as specified by a user-supplied routine. Each nuclide dissolves in an amount which is the lesser of the rate at which it is being released by leaching of the waste matrix or its equilibrium solubility in the water flowing through the repository. If the waste canisters are surrounded by clay buffers, the water flow rate used in solubility calculations is adjusted to account for steady-state diffusion through the clay.

If the leaching of the waste form takes less time than is required for the water content of the repository to flush out, the rate at which any nuclide can leave the repository is reduced to

$$\Lambda_e = \frac{Q_s}{Men\ a} \tag{8.29}$$

The code then proceeds to treat the transport of the dissolved radionuclides through a network of flow paths. The heads h at each node of the network are either input or calculated by simultaneously solving for all legs the equation

$$q_{ji} = \frac{1}{R_{ij}} [h_i - h_j] \tag{8.30}$$

and

$$\sum_{i \neq j} q_{ji} = 0 \tag{8.31}$$

where q_{ji} is the flow from node i to node j and R_{ij} is a "hydraulic resistance" given by

$$R = \frac{L}{KA} \tag{8.32}$$

where L is the path length, K is the hydraulic conductivity, and A is the cross-sectional area. The pore velocity of the water is then

$$V = \frac{q}{An} \tag{8.33}$$

where n is the effective porosity.

Transport through each path segment is calculated by means of a function which is the amount (normalized by Equation 8.26) of a given contaminant which emerges from the outlet of the path segment during time interval ℓ. This is obtained by a Green's function method:

$$F_\ell = \sum_{\ell' \leq \ell} F'_{\ell'} G_{\ell'\ell} \tag{8.34}$$

where F'_ℓ is the normalized amount <u>entering</u> the pipe during time interval ℓ'. The Green's function G is given by

$$G_{\ell'\ell} = \tfrac{1}{2}\left[g(T_{\ell+1} - T_{\ell'}) - g(T_\ell - T_{\ell'})(1 - \delta_{\ell'\ell})\right] \tag{8.35}$$

$$g(t) = \operatorname{erfc}\left\{\frac{L - \frac{V}{B}t}{\sqrt{\frac{4\alpha V t}{B}}}\right\} - e^{L/\alpha} \operatorname{erfc}\left\{\frac{L + \frac{V}{B}t}{\sqrt{\frac{4\alpha V t}{B}}}\right\} \tag{8.36}$$

where T_ℓ is the time at which interval ℓ begins, δ is the Kronecker delta function, B is the retardation factor, and is the dispersivity.

In order to avoid numerical problems, a number of alternative forms of Equation (8.26) derived from the asymptotic expansion of the complementary error function are employed in certain circumstances.

When flow paths branch, the contaminant is divided in proportion to the water flow.

The concentration of contaminant in well water may be calculated from two models. In the limit of a large withdrawal rate, all contaminated water will discharge through the well. In this case Equations (8.34) - (8.36) are used with the aquifer velocity corrected to account for pumpage.

In the limit of small withdrawal rate, the well will sample the concentrations of contaminants which would be present in the absence of the well. In this case, a two-dimensional analog of Equations (8.34) - (8.36) is used. Lateral dispersion is accounted for and contaminants may enter the aquifer at any number of points.

At the conclusion of the calculations, release rates of nuclides not formed by decay of a parent are found from Equation (8.26). In the case of decay chains, the normalized release rate of the daughter is found by multiplying the normalized release rate of the parent by a correction factor which depends on the hydrologic parameters in the leg closest to the point of release. The correction factor R is given by

$$R = B_1/B_2 \tag{8.37}$$

for peak release rates and by

$$R = \frac{B_1(\lambda_1 - \lambda_2)\,(e^{r_2 L} - e^{r_1 L})}{(B_1\lambda_1 - B_2\lambda_2)\,(e^{r_* L} - e^{r_1 L})} \tag{8.38}$$

for releases integrated over all time, where the subscripts 1 and 2 denote parent and daughter, respectively, λ denotes half life (yr), and

$$r_j = \frac{1 - \sqrt{1 + 4\alpha B_j \lambda_j / V}}{2\alpha} \qquad j = 1,2 \tag{8.39}$$

$$r_* = \frac{1 - \sqrt{1 + 4\alpha B_1 \lambda_2 / V}}{2\alpha} \tag{8.40}$$

Changes in ground-water flow are treated by allowing the system to change state. Heads, permeabilities, etc. can take different values in different states. The transition between states corresponds to an "event"; continuous changes must be approximated by one or more discrete events.

NUTRAN can account for events in three different ways:

- Scenarios in which events occur at specified times can be modeled.
- Events can be taken to occur at times specified by random numbers. The resulting scenarios are then modeled and the outputs analyzed statistically. Use of this method requires additional statistical software which is not part of NUTRAN.
- Expected values of doses and radionuclide concentrations can be calculated directly using the occurrence rates of the events.

When the third of these methods is used, the quantity F_ℓ is replaced by $F_{\ell n}$, the expected amount of contaminant emerging from the path segment if the system is in state n, multiplied by the probability of being in state n. Equation (8.34) then becomes

$$F_{\ell n} = \sum_{n'} \sum_{\ell' \leq \ell} F'_{\ell' n'} G_{\ell' \ell} \psi_{n' n} \qquad (8.41)$$

where G is calculated as if the system were in state n' and the matrix of ψ is given by

$$\psi = e^{-P(T_\ell - T_{\ell'})} \qquad (8.42)$$

where P is a matrix whose elements are the rates of transition among the states.

Numerical Approximations - The principal numerical approximations in WASTE and PLOT are as follows:

- Flow of fluid is usually approximated by a network of one-dimensional paths.
- The transport equation in each leg is solved using boundary conditions which would be appropriate if the leg were infinitely long.
- The input to each leg is approximated by a series of discrete instantaneous pulses.
- The Green's function for a two-dimensional aquifer is integrated numerically.
- Wells have either a withdrawal rate so small as to have no effect on the aquifer from which they draw or one so large that they function as interceptor wells.

- Time required for water to enter surrounding rocks as the repository repressurizes is treated very approximately.

- Equilibrium solubility limits are calculated for the most abundant radioactive isotope of each element only; other radioisotopes are assumed to dissolve in the same proportion.

- The rate of release of each radionuclide into ground water is given by the slowest of the relevant processes; if two processes proceed at comparable rates, their effects are not combined.

- Radionuclide chains are incorporated by use of correction factors which are not always correct (although they always give upper bounds for the peak and total releases).

- When the water velocity changes, atoms continue to move at the old velocity until they reach the end of the flow leg they are in.

Probabilistic or Statistical Aspects - If discrete changes in water velocity or the opening of new flow paths can occur at any time, the code will use Equation 8.42 to calculate expected values of radionuclide releases from the occurrence rates of these events. The code can also be run repetitively to calculate expected values by a Monte Carlo method.

Assumptions and Simplifications - The principal assumptions, other than those listed above as numerical approximations, are as follows:

- 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.

- Water in waste storage rooms is well mixed.

Structure and Level of Detail - 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.

Major Dependent Variables - The key variable in WASTE is the normalized flow which is calculated from Equation (8.34) or (8.41). Other variables are listed in the section on equations.

Applicability, Limitations, Validity, and Completeness - The model is applicable to a wide variety of cases, including some not handled well by finite-element and finite-difference methods. The principal limitation is the requirement that the flow field be represented by a network of one-dimensional path segments.

References -

1. Ross, B., C.M. Koplik, M.S. Giuffre, and S.P. Hodgin, "A computer model of long-term hazards from waste repositories," Radioactive Waste Management, Vol. 1, pp. 325-38, 1981.

2. Ross, B., C.M. Koplik, M.S. Giuffre, S.P. Hodgin, and J.J. Duffy, "NUTRAN: A computer model of long-term hazards from waste repositories," The Analytic Sciences Corporation Report UCRL-15150, December 1979.

3. Ross, B. and C.M. Koplik, "A new numerical method for solving the solute transport equation," Water Resour. Res., Vol. 15, pp. 949-55, 1979.

4. Giuffre, M.S. and B. Ross, "The effect of retardation factors on radionuclide migration," in G.J. McCarthy, ed., Scientific Basis for Nuclear Waste Management, Vol. 1, pp. 439-442, Plenum, New York and London, 1979.

5. Ross, B. and C.M. Koplik, "A statistical approach to modeling transport of pollutants in ground water," Mathematical Geology, Vol. 10, pp. 657-672, 1978.

6. Berman, L.E., D.A. Ensminger, M.S. Giuffre, C.M. Koplik, S.G. Oston, G.D. Pollak, and B.I. Ross, "Analysis of some nuclear saste management options," The Analytic Sciences Corporation Report UCRL-13917, October 1978.

7. Ross, B., C.M. Koplik, M.S. Giuffre, S.P. Hodgin, J.J. Duffy, and J.Y. Nalbandian, "User's Guide to NUTRAN: A computer analysis system for long-term repository safety," Atomic Energy of Canada, Ltd., Technical Record AECL-TR-121, September 1980.

8.7 AT123D Area: Repository Siting

I. Summary of Code

Purpose and Scope - AT123D (Analytical Transient 1-, 2-, or 3-Dimensional) provides analytic or Green's Function solutions to the solute transport equation in 1, 2, or 3 dimensions with a constant uniform water velocity.

Author - AT123D was written by G.T. Yeh at Oak Ridge National Laboratory.

Code Functions - The program provides solutions in 1, 2, or 3 dimensions. 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 ground water.

Potential Usage - AT123D requires that the water flow be known and be approximated by a uniform parallel flow. The calculated concentrations may be used to check compliance with EPA guidance if the aquifer lies within the accessible environment; however, such calculations must be preliminary in nature due to the restrictive assumptions incorporated in the code. The code might also be useful for benchmarking more complex codes.

Related NRC Issues (See Table 1-4) - 3, 7, 8, and 40.

Restrictions - None; the program has been published.

II. Summary of Findings

General Critique - AT123D could be useful as a tool for preliminary evaluations, which is its intended use. The many limitations of the code necessitate use of another code for final evaluation of a site. It could also be used to check the accuracy of more complicated programs.

For one-dimensional problems, especially when one is interested in releases to the surface rather than concentrations in ground water, GETOUT will usually be preferable to AT123D because it incorporates decay chains. The primary use of AT123D will be when one is concerned with lateral dispersion in an aquifer.

In all cases except for instantaneous releases, AT123D performs a numerical integration over time. It is not clear what constraints there are on the choice of time step for this integration.

Applicability to Medium - AT123D is applicable to any medium, but only to systems which can be approximated by constant uniform parallel flows.

Sensitivity Analysis - Yeh presents results of 50 cases in the User's Manual (ref. 1).

Code Verification - The code has been checked against hand calculations and laboratory experiments.

Field Validation - None.

III. General Description

Operating Characteristics - AT123D is written in FORTRAN IV, and should be adaptable to most computers.

Inputs - The principal inputs are as follows:

Location and dimensions of the source
Aquifer dimensions
Porosity
Hydraulic conductivity
Hydraulic gradient
Dispersivity
Distribution coefficient
Duration of release

Outputs - The output of the code is a series of tables showing concentration at selected points and selected times.

Available Documentation - A user's manual has been published. It documents the theory of the code and input/output formats in an acceptable manner. It also includes a listing of the program, but does not document it.

IV. Review of Theory

Equations - AT123D solves the solute transport equation in the form:

$$B \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i} D_{ij} \frac{\partial C}{\partial x_j} - \frac{\partial}{\partial x_i} V_i C - \lambda BC + \frac{Q}{\phi} \qquad (8.43)$$

where C is concentration, B is the retardation factor, D is the dispersion coefficient, V is pore velocity, λ is a radioactive decay constant, Q is the rate of release, and ϕ is effective porosity.

The solution is given by separating the spatial variables and obtaining Green's functions of time:

$$C(x,y,z,t) = \int \frac{Q(\tau)}{\phi} X(x,t;\tau)\, Y(y,t;\tau)\, Z(z,t;\tau)\, d\tau \qquad (8.44)$$

The form of the functions X, Y, and Z depends on whether there are boundary conditions imposed at planes perpendicular to the respective direction. When boundaries are present, the functions are represented by infinite sums; when the boundaries are at infinity, the functions have a closed form.

The formulas for X, Y, and Z are quite lengthy and will not be presented here; they are given by Yeh in the User's Manual.

The integral over τ is carried out numerically.

Numerical Approximations - The principal numerical approximations in AT123D are the following:

- Numerical integration over time
- Truncation of infinite sums in cases with boundary conditions
- Dispersivity tensor has principal axes aligned with the flow.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - 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
- Release of contaminant at a constant rate over some duration.

Structure and Level of Detail - AT123D is simple; it assumes uniformity within a rectangularly shaped area.

Major Dependent Variables - The code solves for concentration.

Applicability, Limitations, Validity, and Completeness - 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.

References -

1. Yeh, G.T., "AT123D: Analytical transient one-, two-, and three-dimensional simulation of waste transport in the aquifer system," Oak Ridge National Laboratory Report ORNL-5602, March 1981.

8.8 KONBRED Area: Repository Siting

I. Summary of Code

Purpose and Scope - KONBRED simulates ground-water 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.

Authors - 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.

Code Functions - KONBRED solves the ground-water 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.

Potential Usage - KONBRED's greatest value will be in studying heterogeneous aquifers overlying specific well-explored sites. Its transient features could also be useful in evaluating the consequences of severe hydrologic stresses such as catastrophic floods or the advance or retreat of glaciers.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - The code has been published and is available to the public.

II. Summary of Findings

General Critique - KONBRED is a well-tested and well-documented code that would be well-suited for solving single-aquifer problems. Its high degree of acceptance makes it stand out among solute transport codes used in waste repository studies.

A principal disadvantage is that nodes must be placed in an equally spaced rectangular array.

The original code treats only conservative solutes; however, a modified version has recently been completed (ref. 5) for application to radioactive waste problems. The new version considers radioactive decay, but does not consider formation of daughter products. It is restricted to equilibrium adsorption (either linear or nonlinear).

Given the requirement of equal spacing of nodes and the limitations of the iterative ADI solution technique, combined with the greater permeability contrasts and longer time scales encountered in high-level radioactive waste analysis, it may be difficult to apply KONBRED.

Applicability to Medium - The aquifers to which KONBRED is applicable might be found near any medium used for a repository.

Sensitivity Analysis - The code has had extensive sensitivity analysis performed on it, involving both physical and numerical parameters (see ref. 1).

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.

Field Validation - 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 build-up in a stream-aquifer system (ref. 3), and (3) radionuclide transport at INEL (ref. 4).

Whether such studies constitute a real field validation of this or any other solute transport model is a controversial question. The solute transport models contain adjustable parameters (such as dispersivity) which cannot be independently measured. It can be argued that manipulation of these parameters would allow the models to simulate almost any observed data.

III. General Description

Operating Characteristics - 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.

Inputs - The principal inputs to the original version 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 concentration at each injection well
Pumping period

The revised version requires additional inputs describing sorption and radioactive decay.

Outputs - The principal outputs are the heads and concentrations. These can be printed out either after each time step at up to five "observation wells" or at all nodes after each 50 time steps.

Available Documentation - The code is documented (ref. 1). The computer card deck of the original code can be obtained, at cost, by requesting it from:

Ralph N. Eicher
Chief, Office of Teleprocessing
Mail Stop 805, National Center
U.S. Geological Survey
Reston, Virginia 22092

The modifications are documented in Ref. 5.

IV. Review of Theory

Equations - KONBRED has two parts, the calculations of water flow and solute transport.

Water flow is calculated by first computing the hydraulic head field h at each time step from a finite-difference approximation to:

$$\frac{\partial}{\partial x_i}\left(T_{ij}\frac{\partial h}{\partial x_j}\right) = S\frac{\partial h}{\partial t} + W \qquad i,j = 1,2 \tag{8.45}$$

where

T	is the transmissivity tensor,
S	is the storage coefficient, and
W(x,y,t)	is the volume flux per unit area.

Equation (8.45) is solved for each node at a given time step by an alternating direction implicit procedure. The flux W is obtained from

$$W(x,y,t) = Q(x,y,t) - \frac{K_z}{m}(H-h) \tag{8.46}$$

where

Q	is the rate of withdrawal or recharge through wells,
K_z	is the vertical hydraulic conductivity of the confining layer,
m	is the thickness of the confining layer, and
H	is the hydraulic head in the source bed, stream, or lake.

The water velocity is found from the head gradient:

$$\vec{V} = \frac{1}{\varepsilon} K \cdot \vec{\nabla} h \tag{8.47}$$

where K is the hydraulic conductivity tensor, ε is the effective porosity, and the head gradient is found by taking the difference between values at adjacent nodes.

Solute transport is solved by the method of characteristics. In this method, several particles are placed within each cell. In each time step each particle is moved to a new position

$$\vec{x}' = \vec{x} + \vec{V}\Delta t$$

where Δt is the duration of the time step.

An interim concentration C* within each cell is then calculated by averaging the concentrations corresponding to the particles which lie within the cell after being moved. The new concentration C' is computed by adjusting this interim concentration to account for dispersion, external fluid sources, and changes in saturated thickness. This adjustment is given by

$$C' = C^* + \Delta t \left[\frac{1}{b} \frac{\partial}{\partial x_i} \left(b\, D_{ij} \frac{\partial C}{\partial x_j} \right) + F \right] \tag{8.48}$$

$$F = \frac{1}{\varepsilon b} \left[C \left(S \frac{\partial h}{\partial t} + W - \varepsilon \frac{\partial b}{\partial t} \right) - C_w W \right] \tag{8.49}$$

where b is the aquifer thickness and D is the dispersion tensor. The concentration C used in these formulas is the average of the interim concentration C* and the concentration in the cell computed in the previous time step. If water is entering the aquifer ($W < 0$), C_w is equal to the concentration of solute in the source fluid; if water is leaving the aquifer ($W > 0$), C_w is equal to C.

For the new version, the concentration is appropriately modified to account for sorption and/or decay.

Equation (8.48) is solved by an explicit finite-difference calculation. If C' exceeds C*, the concentration associated with each particle in the cell is increased by the amount C' - C*. If C* exceeds C', the concentration of each particle is multiplied by the factor C'/C*.

Numerical Approximations - The principal numerical approximations in KONBRED are the following:

- Discretization of space and time
- Off-diagonal elements of the transmissivity tensor are neglected
- Particle velocity is constant over each time step rather than following curved streamlines
- Concentrations are averaged over a cell before solving Equation (8.48)
- Dispersion and recharge occur in "bursts" at the beginning of each time step rather than continuously
- Constant-head boundaries are approximated by zones of high leakance.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The main assumptions are:

- 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.

Structure and Level of Detail - 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.

Major Dependent Variables - The major variables, other than the inputs, are the heads, water velocities, and concentrations.

Applicability, Limitations, Validity, and Completeness - The code was designed to simulate solute transport in two dimensions. For this problem, it is complete and widely accepted as valid. Even with the restriction to two dimensions, it has a wide range of applicability. The principal limitations are:

- Decay chains with more than one member are not treated.
- Nodes must be equally spaced in each direction (although the spacing in the two coordinate directions may be different).
- The node network can be no larger than 20 by 20. The program can and should be modified to change this limit.
- Iterative ADI is used to solve flow equation.

References -

1. Konikow, L.F. and J.D. Bredehoeft, Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water, Techniques of Water-Resources Investigations of the United States Geological Survey, Book 7, Chapter C2, 1978.

2. Konikow, L.F., "Modeling chloride movement in the alluvial aquifer at the Rocky Mountain Arsenal, Colorado," U.S. Geol. Survey Water-Supply Paper 2044, 1977.

3. Konikow, L.F. and Bredehoeft, J.D., "Modeling flow and chemical quality changes in an irrigated stream-aquifer system," Water Resour. Res., Vol. 10, No. 3, p. 546-562, 1974.

4. Robertson, J.B., "Digital modeling of radioactive and chemical waste transport in the Snake River Plain aquifer at the National Reactor Testing Station, Idaho," U.S. Geol. Survey Open-File Rept. IDO-22054, 1974.

5. Tracy, J.V., "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, 1982.

8.9 FEMWASTE Area: Repository Siting

I. Summary of Code

Purpose and Scope - FEMWASTE (A Finite-Element Model of Waste Transport Through Saturated-Unsaturated Porous Media) was developed to compute waste transport through porous media under dynamic ground-water conditions.

Authors - 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 (ref. 2).

Code Functions - This finite-element model of waste transport through porous media simulates the spatio-temporal distribution of both the waste concentration and flux under dynamic ground-water conditions. The system may have both saturated and unsaturated regions. The transport mechanisms include advection, hydrodynamic dispersion, chemical sorption, and first-order decay.

The aquifer to be modeled may be described in areal or cross-sectional coordinates. The aquifer parameters may be distributed or zoned, and the system may be anisotropic. The model considers sorption. This is taken into account by the introduction of a retardation factor into the governing mass-balance equation. Nonlinearities are also considered insofar as the bulk density, and consequently the retardation factor, are a function of the moisture content. The velocity field is required as part of input to this model. FEMWATER, the companion to FEMWASTE, produces this required velocity field.

Potential Usage - FEMWASTE is capable of a two-dimensional simulation of the transport of contaminants in an aquifer system. FEMWASTE is considered a far-field code in the sense that the flow and transport is analyzed outside the disturbed zone.

Related NRC Issues (See Table 1-4) - 3, 7, 8, and 40.

Restrictions - The code is public and is therefore available to the NRC.

II. Summary of Findings

General Critique - If transport in the unsaturated zone is important, then this code would be appropriate. If this is not the case, however, the other codes described in this section would be preferable because of numerical inefficiencies introduced by the numerical method and by considering the extra flow condition.

FEMWASTE is an extension of the work performed by Duguid and Reeves (ref. 2) in which the mass balance equation governing the concentration distribution is solved by the Galerkin finite-element method subject to appropriate initial and boundary conditions. FEMWASTE uses a technique known as upstream weighting. This has a distinct advantage over the

Galerkin formulation when analyzing advection-dominated transport because it reduces the numerical oscillations associated with the Galerkin method.

Applicability to Medium - FEMWASTE is designed to simulate contaminant transport in a saturated or unsaturated porous medium subject to variable boundary or initial conditions. The code is applicable to most porous media as long as a two-dimensional simulation is valid.

Sensitivity Analysis - A sensitivity analysis was performed on the numerical schemes by running the code for the same physical problem and comparing results for the ten alternative numerical schemes that are provided.

Code Verification - A sample problem of transport from a seepage pond reported by Duguid and Reeves (ref. 2) 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 (ref. 4).

Field Validation - None.

III. General Description

Operating Characteristics - FEMWASTE is written in FORTRAN IV for use on an IBM 360 computer.

Inputs - Inputs for FEMWASTE include:

Distribution coefficient
Bulk density
Longitudinal and transverse dispersivities
Decay constant
Porosity for each material
Modified coefficient of compressibility for each material
Nonlinearity effects of any of the above with moisture content
Initial conditions
Boundary conditions
Geometrical data
Fluid properties

Outputs - Output for FEMWASTE consists of the concentration distribution at each time step.

Available Documentation - FEMWASTE is documented in ref. 1.

IV. Review of Theory

Equations - The governing equations to describe the distribution of a pollutant constituent in a two-dimensional subsurface porous system is obtained from the law of mass balance. This can be written in the form

$$L(c) = \frac{\partial}{\partial t}(\theta c + \rho s) + (\theta c + \rho s)\alpha' \frac{\partial h}{\partial t} + \left(\frac{\partial V_x c}{\partial x} + \frac{\partial V_z c}{\partial z}\right)$$

$$- \left[\frac{\partial}{\partial x}\left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xz} \frac{\partial c}{\partial z}\right) + \frac{\partial}{\partial z}\left(\theta D_{zx} \frac{\partial c}{\partial x} + \theta D_{zz} \frac{\partial c}{\partial z}\right)\right]$$

$$+ \lambda(\theta c + \rho s) - M = 0 \qquad (8.50)$$

where θ is the moisture content; c is the concentration of dissolved constituent in the water; ρ is the bulk density of the solid; s is the concentration of the constituent that is adsorbed on the solid; α' is the modified coefficient of compressibility of the medium; h is pressure head of the water; D_{xx}, D_{xz}, D_{zx}, and D_{zz} are the dispersion-coefficient tensor components; V_x and V_z are the Darcian velocity components in the x- and z-directions, respectively; λ is the decay constant; M is the artificial source; x and z are the horizontal and vertical coordinates, respectively; t is the time; and L is an operator.

The dispersion-coefficient tensor may be related to flow-field and media properties as (ref. 2)

$$\theta D_{xx} = a_T V + (a_L - a_T)V_x^2/V + D_m T$$

$$\theta D_{xz} = \theta D_{zx} = (a_L - a_T)V_x V_z/V$$

and

$$\theta D_{zz} = a_T V + (a_L - a_T)V_z^2/V + D_m T \qquad (8.51)$$

where $V = \sqrt{V_x^2 + V_z^2}$; a_T and a_L are the transverse and longitudinal dispersivities, respectively; T is the tortuosity; and D_m is the molecular diffusion coefficient. The decay constant, λ, is a property of the constituent and ρ and α' are the properties of the porous media under consideration. The independent variables include: x,z, and t. Thus, there are two dependent unknowns, c and s, in Equation (8.50) to be determined. An additional equation is required to completely define the system. It is assumed that the adsorption of the constituent by the solid is to occur at a rapid rate (i.e., a fast exchange reaction) such that the dissolved material is in equilibrium with the material adsorbed by the solid. This is expressed by the linear equation:

$$s = K_d c \qquad (8.52)$$

where K_d is the distribution coefficient. Thus Equation (8.50) may be rewritten as:

$$L(c) = \theta R_d \frac{\partial c}{\partial t} + \left(\frac{\partial V_x c}{\partial x} + \frac{\partial V_z c}{\partial z}\right) - \left[\frac{\partial}{\partial x}\left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xz} \frac{\partial c}{\partial z}\right)\right.$$

$$\left. + \frac{\partial}{\partial z}\left(\theta D_{zx} \frac{\partial c}{\partial x} + \theta D_{zz} \frac{\partial c}{\partial z}\right)\right] + \left(\frac{\partial \theta}{\partial t} + \alpha' \theta R_d \frac{\partial h}{\partial t} + \lambda \theta R_d\right)c - M = 0 \quad (8.53)$$

where

$$R_d = 1 + \frac{\rho K_d}{\theta} \quad (8.54)$$

is the retardation factor, which is a measure of the delay of the breakthrough of the dissolved constituent.

The initial condition of Equation (8.53) is assumed to be known as:

$$c = c_o(x,z) \qquad \text{at } t = 0 \text{ and } (x,z) \text{ in } R, \quad (8.55)$$

where c_o is a given function of spatial coordinates, x and z; R is a region bounded by the curve, $B(x,z) = 0$. This c_o may also be obtained by simulating the steady version of Equation (8.53) with steady boundary conditions and ground-water flow field.

Three types of boundary conditions may be specified depending on the physical constraint. The first one is the Dirichlet boundaries on which the concentration is prescribed. The second one is the Cauchy boundaries on which the normal gradient of the concentration is prescribed. The third type, Neumann boundary conditions, is a degeneration of the Cauchy boundary condition when it is applied to the flow through boundaries with inflows into the region. The three boundary conditions are given as

(1) The Dirichlet boundary condition

$$c = c_1(x,z,t) \quad \text{on } B_1 \quad (8.56)$$

where B_1 is a portion of B, and c_1 is a given function of time and (x,z) on B_1.

(2) The Cauchy boundary condition

$$-\left(\theta D_{xx} \frac{\partial c}{\partial x} + \theta D_{xz} \frac{\partial c}{\partial z} - V_x c\right)n_x - \left(\theta D_{zx} \frac{\partial c}{\partial x} + \theta D_{zz} \frac{\partial c}{\partial z} - V_z c\right)n_z$$

$$= q_2(x,z,t) + (V_x n_x + V_z n_z)c \quad \text{on } B_2 \ , \quad (8.57)$$

where n_x and n_z are the directional cosines of the outward unit vector normal to the B_2 portion of the curve B; $q_2(x,z,t)$ is the given function of time, t, and (x,z) on B_2.

(3) The Neumann boundary condition

$$- (D_{xx}\theta \frac{\partial c}{\partial x} + D_{xz}\theta \frac{\partial c}{\partial z} - V_x c)n_x - (D_{zx}\theta \frac{\partial c}{\partial x} + D_{zz}\theta \frac{\partial c}{\partial z} - V_z c)n_z = q_3(x,z,t) \quad \text{on } B_3 \ , \tag{8.58}$$

where q_3 is a given function of time and points (x,z) on B_3 portion of B.

Numerical Approximations - Equations (8.53) through (8.58) are integrated in the spatial dimensions by the weighted-residual method in conjunction with finite elements. The region of interest is subdivided into an assemblage of smaller sub-domains called elements. Following the procedure of finite-element weighted-residual method, and employing quadrilateral bilinear elements for spatial discretization, an approximate formulation of the concentration distribution, c, is obtained.

The finite-difference methods are typically used in the approximation of the time derivative. Three time-marching methods are adopted in the present model. In the first one, the central or Crank-Nicolson formulation is used, in which the required matrices are evaluated at $t + \Delta t/2$. In the second method the backward difference formulation is used in which the required matrices are evaluated at $t + \Delta t$. In the third optional method, the values of the unknown variables are assumed to vary linearly with time during the time interval, Δt. In this mid-difference method, the required matrices are all evaluated at $t + \Delta t/2$. This option has been shown superior to the central or backward-difference formulation, if the mass matrix is not lumped.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The major assumptions are:

- Validity of the solute transport equation for unsaturated flows.
- Sorption may be represented as equilibrium adsorption.
- The distribution coefficient, K_d, is independent of moisture content.
- Bulk density, ρ_e, is dependent on moisture content.

Structure and Level of Detail - The porous medium is represented by a two-dimensional grid. The domain is discretized using noded isoparametric finite elements of almost any quadrilateral shape. The shape functions may be bilinear or may include upstream weighting coefficients.

Major Dependent Variables - Aside from the input parameters, the major variables are the nodal contaminant concentrations.

Applicability, Limitations, Validity and Completeness - A significant limitation in the use of this model is the fact that a two-dimensional simulation only may be performed. However, in many cases of bedded formations, the two-dimensional model would prove to be adequate. Unlike the other solute-transport codes discussed here, FEMWASTE can model problems involving the unsaturated zone.

References -

1. Yeh, G.T. and S.D. Ward, "FEMWASTE: A finite-element model of waste transport through saturated-unsaturated porous media," Oak Ridge National Laboratory Report ORNL-5601, 1981.

2. Duguid, J.O. and M. Reeves, "Material transport through porous media: A finite-element Galerkin model," Oak Ridge National Laboratory Report ORNL-4928, 1976.

3. Bear, J., Dynamics of Fluids in Porous Media, American Elsevier, New York, 1972.

4. Reeves, M. and J.O. Duguid, "Water movement through saturated-unsaturated porous media: A finite-element Galerkin model," Oak Ridge National Laboratory Report ORNL-4927, 1975.

8.10 PATHS Area: Repository Siting

I. Summary of Code

Purpose and Scope - PATHS is a two-dimensional preliminary analysis tool to determine the movement of water-transported contaminants accidentally released from a waste storage facility.

Authors - Written by R.W. Nelson and J.A. Schur, PATHS was a result of research conducted by Pacific Northwest Laboratory and supported by the Waste Isolation Safety Assessment Program (WISAP).

Code Functions - The basis of the code is a two-dimensional analytical solution for the ground-water potential distribution. From the potential distributions the pathline differential equations are written and then numerically solved by the code to give the paths of the fluid particles and their advance with time toward the outflow boundary. It is essentially an idealized hybrid analytical/numerical model for two-dimensional, saturated ground-water flow and single component transport in homogeneous geology.

The model treats both steady and transient saturated flow systems. Wells may also be present. Geochemical retardation is considered, but dispersion is ignored.

Potential Usage - PATHS was designed to enable estimates of expected contaminant-transport consequences when limited field data are available. Accordingly, the model is necessarily simplified and idealized as the representation of the real situation. However, special care was exercised to assure that minimum worst-case estimates for the fluid travel times would be provided by the model.

The model may also be used as a verification tool in which the analytical solution of PATHS may calibrate the results produced by more general numerical models. PATHS is most useful for examining conditions in the regional area.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - The code is public and therefore available to the NRC.

II. Summary of Findings

General Critique - PATHS has two distinct uses, as a preliminary analysis tool and as a verification tool to calibrate results of more general numerical models.

A preliminary analysis commonly is restricted by lack of field data. In particular, there is insufficient hydraulic conductivity, porosity, or stratum configuration data to enable a detailed description of the actual field situation. Accordingly, the approach used here involves idealizing the model to keep it within the available data bounds, followed by selecting conservative alternatives at decision points to assure that the predicted results will represent a worst-case situation. The code, although idealized, provides a fast, inexpensive first-cut evaluation tool, consistent with the amount of field data usually available.

To obtain an accurate analysis of a flow field in a real situation, a multi-dimensional model may eventually be required to take into account the anisotropy and non-homogeneity of the system. These models may be numerical models with corresponding mathematical approximations. It is important that these models be calibrated with some known analytical solutions so that the accuracy of the model may be determined and a corresponding mesh size or block size may be designed for the required accuracy. PATHS is a model that uses these analytical solutions.

The model assumes no dispersion effects. This does not necessarily yield the worst overall result in terms of the amount of contaminants reaching the biosphere and so is a distinct disadvantage in the use of this model in a real situation.

Additionally, the simplifications in this model restrict the use to a small number of engineering situations.

A further problem is that the code appears to be usable only on certain computer equipment.

Applicability to Medium - With the simplifying assumptions incorporated, PATHS is restricted in use to a uniform thickness, horizontal, confined, isotropic, homogeneous aquifer system. There are situations where these assumptions are acceptable.

Sensitivity Analysis - Several examples cases appear in the PATHS user's manual (ref. 1) for a variety of engineering situations.

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.

Field Validation - None.

III. General Description

Operating Characteristics - The code is written in FORTRAN IV and appears to be machine dependent for the UNIVAC 1100/44 at PNL. This machine, however, is available for use by the public.

Inputs - The input data structure of this model is based on hydrogeologic data usually compiled for the ground-water system. Input data preparation may be simplified by the use of a suitable worksheet. This worksheet may be found in the PATHS user's manual (ref. 1). The input parameters consist of aquifer data, boundary conditions, time dependent conditions, pond and well source values.

Outputs - This interactive program is able to produce results in tabular form or in the form of computer plots. The output consist of contaminant arrival results, fluid pathlines and advancing fronts, location/arrival time distribution and location/outflow quantity distribution.

Available Documentation - PATHS is documented in Ref. 1.

IV. Review of Theory

Equations - The model represents flow in a confined stratum of uniform vertical thickness and of large lateral extent in the horizontal plane. The stratum is assumed homogeneous, having isotropic hydraulic conductivity and constant effective porosity. A uniform lateral flow gradient is assumed within the stratum, and the superimposed leakage is from a vertical, cylindrical pond or cavern that completely penetrates the entire stratum. A head is applied at the pond or structure and is completely dissipated at finite radial distance rather than at an infinite distance, thereby introducing a worst-case situation into the evaluation procedure.

The model allows as many as 35 wells at optional locations. Wells are represented as completely penetrating, vertical line sources with steady or time-dependent flow rates.

The model treats both steady and transient saturated-flow systems. The steady-state cases are evaluated by holding the uniform gradient, the head in the pond, and the well strengths constant.

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 model also considers the effect of equilibrium ion-exchange reactions for a single contaminant at trace concentration. The approximate equilibrium coefficient, or K_d approach is utilized to give the ion-exchange delay effects for a single constituent. There are, however, no dispersion effects considered in this model.

The analytic solutions are quite complex and will not be shown here.

Numerical Approximations - The analytic solution used in this code assumes that the distance of the well from the center of the source is much greater than the center to the source boundary. Otherwise, no numerical approximations are used.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal assumptions and simplifications are as follows:

- Fully saturated flow
- Fluid is incompressible
- Velocity field is linear and flow is in steady state
- Two-dimensional horizontal flow
- Confined, isotropic, homogeneous aquifer
- Infinite areal extent
- Uniform potential gradient
- Dispersion effects ignored

Structure and Level of Detail - The code is based on the representation of a potential function formed by a superposition of elementary flows. The overall domain is governed by a uniform potential gradient. However, due to any sources or sinks present, this field may be distorted around such discontinuities.

Any injected contaminants are transported by advection only and no dispersion or diffusion is taken into account.

Major Dependent Variables - The most important variables which are computed or change with time are:

- The potential function
- The stream function
- The concentration

Applicability, Limitations, Validity and Completeness - Due to all the assumptions and simplifications present in PATHS, the code has a very limited application to field problems. However, it is a useful tool in the verification of more general numerical models. PATHS can produce analytic results to more complex engineering problems than can classical analytic solutions.

References -

1. Nelson, R.W. and J.A. Schur, "PATHS groundwater hydrogeological model," Pacific Northwest Laboratory Report PNL-3162, April 1980.

9.0 GEOMECHANICAL CODES

9.1 DNET

Area: Repository Design
Repository Siting

I. Summary of Code

Purpose and Scope - DNET or Dynamic Network model was developed to investigate how water flow near a repository is affected by processes such as salt dissolution and salt creep. It also provides a systematic means for investigating the effects of related processes such as thermal expansion, subsidence, fracture formation, and fracture closure. It treats two-dimensional ground-water flow by a network of one-dimensional flow paths.

Authors - DNET was developed at Sandia National Laboratories and is described in a series of draft reports by R.M. Cranwell, S. Stuckwisch, and J.E. Campbell.

Code Functions - The physical processes that are considered in DNET are: (1) fluid flow through permeable media, (2) salt dissolution, (3) dependence of density and viscosity on temperature and salt concentration, (4) thermal expansion, (5) fracture formation and closure, and (6) salt creep. Submodels are used to represent these various processes; in the code, the submodels are solved sequentially. DNET uses a network flow model.

Potential Usage - DNET is considered a near-field code (i.e., where thermal effects are important). It is designed primarily for examining repositories in bedded salt. It may be used to investigate problems such as (1) dissolution along boreholes and shafts, (2) salt creep, which may tend to close boreholes and shafts, (3) fracture formation and closure, and (4) the flow fields associated with the aforementioned problems. The time-dependent flow network calculated by DNET might be used as an input to a solute-transport code. DNET is most useful for examining conditions in the disturbed zone.

Related NRC Issues (See Table 1-4) - 7, 40, and 44.

Restrictions - The code is available to the NRC and has been released to the public.

II. Summary of Findings

General Critique - The code may be useful for examining some of the problems associated with high-level radioactive storage in salt. The processes that occur in salt are not clearly understood. For example, some fluid flow observations that have occurred during heater experiments in salt have not been adequately explained. Consequently, it is difficult to test completely a model designed to simulate these processes. Because the various processes are solved in a sequential fashion, the code may have time-step restrictions, which are not discussed in the user's guide. The network flow model takes advantage of the one-dimensional nature of a flow field that persists in a geological system of hydraulic layers that vary widely in

permeability. If there is a strong three-dimensional nature to the physical system, however, it is not clear that the DNET code would be applicable. Also, the salt dissolution front seen at some sites would be difficult to analyze with DNET.

A specific network of flow paths (legs and junctions are specified) is built into DNET, and is limited to 18 path segments. This might limit the applicability of the code to sites whose stratigraphy resembles that of the Sandia reference site. Some flexibility is allowed, however, since leg lengths, junction elevations, and leg hydraulic properties can be input. The geometry of the network is similar, but not identical, to that used in NWFT (Network Flow and Transport model). DNET, unlike NWFT, does not calculate solute transport, but it does allow hydraulic properties to vary with time.

DNET requires constant-pressure boundary conditions at the aquifer inlets and discharge points. Consequently, these boundary conditions are valid only if the aquifer inlet and discharge points are sufficiently far removed from the simulated disruption near the repository. This condition may result in additional work, since the network may have to be designed larger than would be expected.

Salt dissolution is modeled by a very simple linear model involving lumped parameters (as opposed to distributed in space). Also, the solubility effects of different mineralogies is not considered. This model requires further justification.

DNET assumes the overlying rock has zero yield stress. The realism of this assumption has been questioned and further examination would be desirable. This is discussed further in the section on assumptions. The deformation aspects of the code, as well as the heat treatment, requires further investigation in order to fully evaluate it.

A minor criticism is that the units used throughout the code are English instead of SI. Finally, from the user's guide, it is not clear how the deformation properties are input.

Applicability to Medium - DNET is designed only for salt applications. The built-in path network corresponds to bedded rather than domed salt. The network corresponds approximately to bedding planes in bedded salt. For domed salt, which has flowed, these bedding planes are probably destroyed, giving the salt a more massive appearance. Therefore, for domed salt, the one-dimensional network approach may not adequately describe the geology. The phenomena the code addresses are only of importance for salt.

Sensitivity Analysis - None reported.

Code Verification - Compared with results from SWIFT for hypothetical problems.

Field Validation - None.

III. General Description

Operating Characteristics - The operating system at Sandia is a CDC 7600. Therefore, DNET was developed on a CDC machine. Conversion to other machines is not anticipated to be difficult. DNET uses two library subroutines, DGEFA and DGESL, that solve systems of linear equations. It is assumed that these subroutines will be made available as part of the DNET code. DNET is programmed in FORTRAN IV.

Inputs - DNET may read single or multiple data sets. In general terms, the input data includes:

Hydraulic conductivity of each leg
Cross-sectional area of each leg
Leg length
Brine concentration
Porosity
Fraction of solubles
Boundary pressures
Junction elevations
Thermal conductivities of each material
Heat capacity of each material
Density of each material
Heat sources
Heat source elevations
Salt properties
Leg-property changes

Outputs - Given the initial conditions, which are input, DNET computes the following: (1) brine concentration, (2) fluid density and viscosity, (3) fluid flow, (4) temperature distribution, and (5) the resulting altered hydraulic properties.

Available Documentation - Documentation for DNET is currently being issued. Sandia National Laboratories are preparing for the NRC a series of manuals that include (1) a user's guide (ref. 1), now available, and (2) self-teaching curriculum (ref. 2).

IV. Review of Theory

Equations - DNET represents the flow field as a network of one-dimensional path segments. It calculates fluid flow through the network, taking account of the following effects:

- Salt dissolution
- Dependence of water density and viscosity on temperature and salt concentration
- Cracking due to stresses induced by thermal expansion and contraction
- Salt creep
- Time dependence of temperature

Fluid flow is calculated during each time step by simultaneously solving in all path segments the equations:

$$q_{ji} = \frac{1}{R_{ij}} \left[P_i - P_j + \rho_{ij} (D_i - D_j) \right] \tag{9.1}$$

and

$$\sum_{i \neq j} q_{ji} = 0 \qquad j = 1, 2, 3 \tag{9.2}$$

where q_{ji} is the flow along the path from node i to node j, P and D are the pressure and elevation at each node, ρ_{ij} is the average fluid density in the path segment, and R_{ij} is a "hydraulic resistance" given by

$$R = \frac{\mu L}{kA} \tag{9.3}$$

where μ is the viscosity of the fluid in the path segment, L is the path length, k is the permeability, and A is the cross-sectional area. Viscosity and density are functions of temperature and salt concentration. Values are obtained from power-series fits to commonly available tables.

Temperature T is obtained by solving the one-dimensional heat equation

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2} + Q(t) \tag{9.4}$$

where α is the thermal diffusivity, with a time-varying heat source. This is equivalent to treating the repository as a uniform infinite plane. The heat source is approximated by a piecewise-linear function of time.

Initial values of salt concentration and cross-sectional area for each path segment must be input. These values are used in the first time step. In each subsequent time step, values calculated in the previous time step are used.

Changes in salt concentration C are given by

$$\frac{dC}{dt} = K_s f_s (C_s - C) \tag{9.5}$$

where K_s is a rate constant governing dissolution, f_s is the mass fraction of soluble material to total solids, and C_s is the saturation concentration of salt. From this equation, DNET estimates the average brine concentration and the quantity of salt removed from each leg undergoing dissolution.

Several processes can change the cross-sectional area of a path segment. These are:

- Salt dissolutioning
- Cracking due to stress caused by thermal expansion and subsidence
- Salt creep.

Changes in cross-section due to dissolutioning are calculated by taking the amount of salt removed from Equation (9.5).

Flow pathways do not necessarily have a specified geometry. A cross-sectional area is required in the input. However, for salt dissolution along a horizontal path, a rectangular cross-sectional area is assumed. Similarly, for dissolution along a vertical path, a circular cross-sectional area is assumed.

The thickness of stress cracks is determined by assuming that stress is confined to a band of width ℓ_o around the repository margin. The total thickness of all the cracks in a layer is set equal to the extension of that layer. The extension is calculated from the Pythagorean theorem; that is, for a net uplift or subsidence of h, the total crack thickness is

$$\Delta\ell = \ell_c^2 + h^2 - \ell_o \qquad (9.6)$$

Salt creep is modeled by calculating the strain rate $\dot{\varepsilon}$ from

$$\dot{\varepsilon} = A\, e^{-Q/RT}\, (\sigma_1-\sigma_3)^n \qquad (9.7)$$

A, Q, and n are empirical parameters, R is the gas constant, and T is the absolute temperature. $\sigma_1 - \sigma_3$ is the deviatoric stress, which is assumed in this model to be equal to the difference between the weight of the overburden and the fluid pressure. In a more recent version, this assumption is relaxed; the resulting treatment of the deviatoric stress is discussed in the section on assumptions and simplifications.

Numerical Approximations - The principal numerical approximations in DNET are the following:

- Pathway dimensions, permeability, fluid density, rock stresses, and temperatures are averaged along each path segment.
- Brine concentrations assumed in each time step are those calculated in the previous time step.
- Viscosity and density are obtained from approximate functional representations.

Probabilistic or Statistical Aspects - The program itself has none. However, it includes a software interface which permits it to be run repetitively in a Monte Carlo mode, if random inputs are generated by another program.

Assumptions and Simplifications - The principal simplifying assumptions (other than those listed above under numerical approximations) are as follows:

- Fluid flow proceeds only along a specified network of 18 path segments.
- Salt dissolutioning follows a first-order rate equation, using quantities averaged across a path segment.
- Pathways have a specified geometry--vertical pathways are cylindrical and horizontal pathways are rectangular.
- Any extension of the overburden occurs by formation of void space in the form of through-going cracks; the yield stress is zero.
- Salt creep follows Equation (9.7) with the stress (when the aperture exceeds a threshold) given by the difference between the overburden weight and the fluid pressure. Below this threshold aperture the effective stress goes linearly to zero. In a more recent version, the treatment of salt creep has been modified to provide a more realistic treatment of the time-dependent nature of the deviatoric stress. The three-dimensional code SANCHO was used to examine stress relief for solution channels and boreholes. The resultant time-dependent estimates of deviatoric stress have been incorporated into DNET. Until the code is obtained for benchmarking, it is not known which version is available.
- Temperature above and below the repository is found by solving the heat equation in one dimension.

Structure and Level of Detail - The code is based on representing the flow field as a network of one-dimensional path segments. The network of repository corridors would be represented as a single path segment. A borehole or shaft could also be represented by a path segment. The code is limited to a specific network of 18 path segments, corresponding to a repository in a salt bed with a simple stratigraphy.

Variable time steps are allowed for increased detail and accuracy in time. An automatic time-step option is also included. The time step can be altered automatically during a calculation in response to changes in fluid-flow rates or changes in hydraulic properties.

Major Dependent Variables - The most important variables describing each path segment, which are computed or change with time, are:

- Temperature
- Salt concentration
- Pressure
- Cross-sectional area and dimensions
- Permeability
- Fluid viscosity
- Fluid density

There are a large number of other variables, most affecting only one of the various processes which DNET treats.

Applicability, Limitations, Validity, and Completeness - The model appears to be complete in including the major phenomena affecting water flow around a bedded salt repository. In this respect, it is unique.

The principal limitation of the code is the restriction to a particular geometry of flow network. This particular geometry describes continuous salt strata and an aquifer above the repository. Extensive reprogramming would apparently be required to use it for sites other than salt beds with continuous strata and an aquifer above the repository.

The least well established assumptions in the program are those regarding stress fracturing and the rate of salt dissolution. Validation of these assumptions is required for the model's predictions to be more credible.

Finally, there are limitations of the code because there are limitations on the data needed to run the code. In particular, data on the following will be difficult to obtain:

K_s - rate constant governing dissolution

f_s - mass fraction of soluble material to total solids

ℓ_o - width of band in which stress is confined

A,Q,n - empirical parameters associated with salt creep model.

References -

1. Cranwell, R.M., S. Stuckwisch, and J.E. Campbell, "DNET user's guide," Sandia National Laboratory Report NUREG/CR-2343, January 1982.

2. "DNET self-teaching curriculum," Sandia National Laboratory, to be published.

9.2 TRUST

Area: Repository Siting

I. Summary of Code

Purpose and Scope - TRUST solves for three-dimensional fluid flow with one-dimensional consolidation in fully saturated and partially saturated systems.

Authors - TRUST was developed by T.N. Narisimhan at the Department of Civil Engineering, University of California, Berkeley. This code grew out of the TRUMP code written by A.L. Edwards.

Code Functions - This model numerically simulates the movement of water in a fully or partially saturated porous media. One of the functions of TRUST is to simulate the compaction of the ground-water reservoir caused by a withdrawal of water. The ground-water reservoir includes those parts of the ground-water system which release water from storage in order to directly compensate for the water withdrawn. If the reservoir occurs at a shallow depth, all the deformations associated with the compaction may be expressed at ground surface as land subsidence. If the reservoir is buried at considerable depths, the effects of compaction may undergo more or less attenuation in being transmitted to the land surface through the overburden. The propagation of the effects of reservoir compaction through the overburden is outside the scope of this model. 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 convenient for handling multidimensional heterogeneous systems composed of isotropic materials.

Potential Usage - This code is very similar to CCC, but the heat transport capability has been replaced by the capability to analyze fluid flow through a partially-saturated porous medium. TRUST could be used to calculate the flow field in situations where subsidence might be significant.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, and 40.

Restrictions - The code is available to the public.

II. Summary of Findings

General Critique - The code simulates flow and deformation in a fully or partially saturated ground-water system. The model combines a general three-dimensional fluid-flow field with a one-dimensional vertical deformation of porous media.

The governing equation is solved by an integrated finite-difference method, using a mixed explicit-implicit iterative procedure to advance in time.

The code would be particularly useful for repositories located near the ground surface, or where excessive ground-water loss may take place. The deformation section of the model would not be applicable for a system with significant overburden between the reservoir and the land surface, if the assumption of one-dimensional consolidation were no longer valid.

Applicability to Medium - The flow segment of the code is generally applicable to most continuous porous media for the three-dimensional simulation of ground-water flow. The deformation segment of the code is applicable when the lateral displacement may be ignored, such as shallow porous-medium systems.

Sensitivity Analysis - Unknown.

Code Verification - In order to verify the model, the five problems listed below were solved:

1. One-dimensional, homogeneous clay column. Step-change in stress, followed by drainage.

2. One-dimensional, heterogeneous clay column. Step-change in total stress, followed by drainage.

3. One-dimensional, homogeneous clay column. Constant total stress. Cyclic variation of hydraulic head at the boundary.

4. Two-dimensional, homogeneous region. Time-dependent total stress with drainage.

5. Axisymmetric, leaky aquifer system. Constant total stress. Pumpage from a well.

Field Validation - Unknown.

III. General Description

Operating Characteristics - TRUST is written in FORTRAN IV and currently exists on UNIVAC and VAX-11 computers. It is also available on the CDC 6400/6600/7000 system at LBL. Unlike the version on UNIVAC, the TRUST programs on VAX do not deal with punch cards. There are two versions of TRUST on the VAX: single and double precisions. Both operate in the same manner.

Inputs - Inputs for TRUST include:

Thickness of flow system
Specific gravity of saturated soil
Well flow rate
Saturation relationship with pore pressure or time
Relative permeability as a function of pore pressure
Coefficient of compressibility
Void ratio as a function of effective stress
Swelling index
Compression index

Outputs - Output for TRUST consists of the pressure distribution, velocity field, saturations, and surface settlement at each time step.

Available Documentation - TRUST is documented in Ref. 3.

IV. Review of Theory

Equations - The governing partial differential equation describing variably saturated flow for an element is:

$$\bar{g} + \frac{\partial}{\partial x_i} V_\ell \cdot \frac{k_{ij}\rho g}{\mu} \frac{\partial}{\partial x_j} (z + \psi) = m_c \frac{D\psi}{Dt} \tag{9.8}$$

in which $\bar{g}$ is the fluid-generation rate per unit volume of the elementary subdomain, V_ℓ is the bulk volume of element ℓ, m_c is specific fluid mass capacity, k_{ij} is the permeability tensor of the medium, ρ is density, g is the acceleration due to gravity, μ is viscosity, z is the elevation, ψ is pressure head and D/Dt is the total derivative. TRUST assumes isotropic conditions, therefore the permeability tensor k_{ij} is the product of the single value of permeability and the kronecker delta ($k_{ij} = k\delta_{ij}$).

The mass conservation may also be reperesented in an integral form as:

$$G_\ell + \int_{\Gamma_\ell} \bar{\rho} \frac{k_{ij}\rho g}{\mu} \frac{\partial}{\partial x_j} (z + \psi) \cdot \phi_i \, d\Gamma = M_{c,\ell} \frac{D\psi_\ell}{Dt} \tag{9.9}$$

in which G is the rate of fluid production from element ℓ bounded by the closed surface Γ_ℓ. $\bar{\rho}$ is the density of the fluid at the surface segment $d\Gamma$, $\bar{k}_{ij}$ is the mean value of the permeability at $d\Gamma$, $M_{c,\ell}$ is the fluid mass capacity of the element ℓ($= m_c V_\ell$) and ψ_ℓ is the mean fluid pressure over element ℓ. In Equation (9.9) k_{ij} and $M_{c,\ell}$ are both functions of ψ, and especially so if the element ℓ is partially saturated.

In partially saturated systems, k_{ij} is to be treated as the product of the relative permeability and the fully saturated or absolute permeability.

The parameters in Equations (9.8) and (9.9) can be functions of space, time or pressure head . The fluid mass capacity is defined as the change in mass per unit increase of pressure head, or

$$M_c = \frac{d}{d\psi} (\rho_w V\phi S) \tag{9.10}$$

$$= SV\phi \frac{\partial \rho_w}{\partial \psi} + \rho_w S \frac{\partial}{\partial \psi} (V\phi) + \rho_w V\phi \frac{\partial S}{\partial \psi} \tag{9.11}$$

where ρ_w is the density of water, ϕ is the porosity, and S is saturation. Parameter M_c represents the mass of fluid which the volume V can absorb due to a unit change in the average value of ψ over V. The three terms on the right-hand side of Equation (9.11) represent the compressibility of water, deformability of the soil skeleton and the desaturability of the pores.

In order for the value of M_c to be evaluated, one needs the constitutive relationships between the pressure head and (1) the fluid density ρ_w; (2) the pore volume $V\phi$; and (3) the saturation S.

The constitutive relationships for all three terms making up M_c are given as:

$$V\phi S \frac{d(\rho_w)}{d\psi} = V_s e S \rho_w \rho_{wo} \beta g, \tag{9.12}$$

$$\rho_w S \frac{d(V\phi)}{d\psi} = \frac{V_s \rho_w S \gamma_w \chi' C_c}{2303\sigma'} \tag{9.13}$$

and

$$V\rho_w \phi \frac{dS}{d\psi} = V_s \rho_w e \frac{dS}{d\psi} \tag{9.14}$$

where

V_s = volume of solid
ρ_{wo} = density of water at atmospheric pressure
γ_w = specific weight of water
β = coefficient of compressibility of water
χ' = $\chi + \psi \, \partial\chi/\partial\psi$
χ = empirical constant

A final expression for M_c may be given as:

$$M_c = V_s \rho_w (Se\rho_{wo}\beta g + S\gamma_w \chi' a_v + e \, dS/d\psi) \tag{9.15}$$

or using C_c instead of a_v

$$M_c = V_s \rho_{wo} (Se\rho_{wo}\beta g + \frac{S\gamma_w \chi' C_c}{2.303\sigma'} + e \frac{dS}{d\psi}) \tag{9.16}$$

where

C_c is the compression index

a_v is the coefficient of compressibility

σ' is the effective stress

e is the void ratio

Note that in Equations (9.14) and (9.15) the quantities ρ_w, s, and e are all functions of ψ and change continuously with time. The parameter $\chi'(S)$ is also a function of ψ, since S is related to ψ.

Numerical Approximations - To numerically solve the governing equations an integrated finite-difference method [IFDM (ref. 2 and 3)] is employed using a mixed explicit-implicit iterative procedure to advance in time.

The central concept of IFDM is to discretize the total flow domain into conveniently small subdomains or "elements" and evaluate the mass balance in each element as indicated in Equation (9.9). Physically, the surface integral on the left-hand side of Equation (9.9) is the summation of fluxes over the surface B and thus measures the rate at which mass is accumulating in the element, as governed by initial and boundary conditions. The right-hand side converts the rate of accumulation of fluid into the corresponding average time rate of change in potential over the element.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The principal simplifications are as follows:

- Terzaghi's theory of one-dimensional consolidation is used; i.e., vertical deformation only is considered; lateral deformation is ignored.
- Darcy's law is valid in both saturated and unsaturated media.
- The pressure depends on the density by an exponential relationship.
- Deformation and saturation are functions of the pore-water pressure head, ψ.

Structure and Level of Detail - The code represents the one-, two-, or three-dimensional system by a rectangular, cylindrical or spherical coordinate system. The domain is discretized by explicitly defined subdomains of the flow region of interest. TRUST is a computer program that implements the equation of mass conservation within such a subdomain.

Within an appropriately small subregion of the flow region (Figure 9-1) over which the variation of ψ is not rapid, the average properties of this volume element are associated with a representative nodal point ℓ. Also, the volume element is so chosen that the lines joining the nodal point ℓ to its neighbors are normal to the interfaces between the

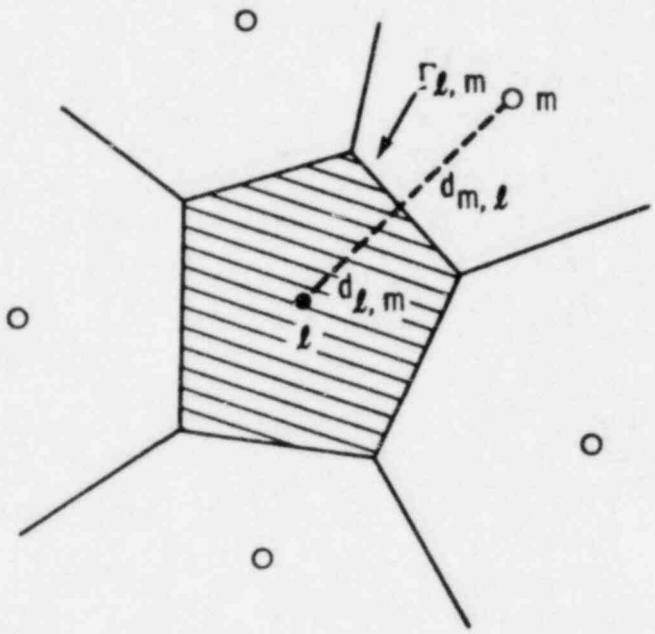

Figure 9-1. Volume Element Associated with Nodal Point ℓ

respective elements. It is assumed that the average properties, such as ψ, associated with each nodal point are functions only of time, while the spatial variation of these average properties between adjacent nodal points can be represented by a simple linear relation which is independent of time.

Major Dependent Variables - The most important variables describing each path segment, which are computed or change with time are:

- Pore-pressure head
- Saturation
- Void ratio
- Relative permeability
- Fluid density
- Effective stress

Applicability, Limitations, Validity, and Completeness - The model appears to be complete in including the major phenomena affecting water flow through fully or partially saturated deforming media.

The principal limitation of the code is the inability of the code to analyze the effects of lateral displacement.

References -

1. Narisimhan, T.N. and P.A. Witherspoon, "Numerical model for land subsidence in shallow groundwater systems," Pub. No. 121 of the Int. Ass. of Hydrologic Sciences, Proc. of the Anaheim Symposium, 1976.

2. Narasimhan, T.N. and P.A. Witherspoon, "An integrated finite difference method for analyzing fluid flow in porous media," Water Resour. Res., Vol. 12, No. 1, p. 57-64, 1976.

3. A.E. Reisenaur, K.T. Key, T.N. Narasimhan, and R.W. Nelson, "TRUST: A computer program for variably saturated flow in multidimensional, deformable media," U.S. Nuclear Regulatory Commission Report NUREG/CR-2360, 1982.

9.3 ROCMAS

Area: Repository Siting
Repository Design

I. Summary of Code

Purpose and Scope - ROCMAS (ROCk MASs) is a finite-element program for the analysis of coupled flow and displacement in deformable, saturated, fractured rock media.

Authors - ROCMAS was developed at Lawrence Berkeley Laboratory, University of California, Berkeley, California by J. Noorishad (ref. 13). ROCMAS is an extension of an earlier code, PORFRC, which was developed by Ayatollahi (ref. 1).

Code Functions - The function of ROCMAS is to provide an analysis of saturated flow and deformation in a fractured porous rock medium. The two-dimensional code combines the capability of isothermal transient pressure analysis and stress-strain analysis in formations with discrete fractures and porous blocks.

Potential Usage - ROCMAS may be considered a near-field or a far-field code. The stress-analysis section of the code may be useful for repository design; however, thermal-mechanical behavior is not incorporated in the present version of the code. The main use to the NRC would be in the analysis of the flow and deformation produced due to water flow in fractured rock or soil within the repository site.

Related NRC Issues (See Table 1-4) - 3, 7, 8, 14, 17, 23, 24, 27, 28, 35, 40, and 44.

Restrictions - The code will be available to the public in the near future.

II. Summary of Findings

General Critique - The code may be useful for the simulation of fluid flow and structural deformation in a fractured porous medium in the region of a nuclear waste repository.

ROCMAS does not now have the capability for thermo-hydromechanical analysis and is not suitable for repository design, as the thermal effects close to the repository play a major role in the stability of the rock medium. However, a thermo-hydromechanical version is under development.

The fractures are modeled discretely, as opposed to the double-porosity or double-continuum approach. The discrete fractures are modeled by incorporating one-dimensional line elements. However, using this method, the exact position, size and direction must be known. Therefore, the fracture-analysis portion of ROCMAS would be severely limited by the availability of data.

Applicability to Medium - ROCMAS is generally applicable to most continuous porous media in which the flow is predominantly two-dimensional (i.e., planar or radial). The fracture flow and deformation section of the code would be applicable to a medium in which the orientation of the discontinuities are known. The code does not contain the capability to analyze a medium in which a statistical average of the number of fractures present in a regional area is known. The double-porosity method could be used under such conditions.

Sensitivity Analysis - Unknown

Code Verification - Most of the efforts to validate this code address the transient fluid-flow behavior in fractures embedded in a porous medium. Validation of the capability to handle coupling between transient fluid flow and stress-strain analysis is limited due to absence of both the analytic solutions and other numerical results. The documented tests (ref. 1) on the transient fluid flow in porous media and in fractures are listed below.

- Continuous Finite-Radius Well Source: The early-time transient-pressure responses of an axisymmetric flow to a producing well are compared with the analytic solution of Mueller and Witherspoon (ref. 11).

- Finite Axisymmetric Aquifer: The late-time pressure responses with no flow as well as constant outer boundaries are compared with the analytic solutions of Muskat (ref. 12).

- Vertical Fractures: The pressure responses for a single vertical fracture and two perpendicular vertical fractures intersecting a well at the center of a rectangular porous medium are compared with the analytic solutions of Raghavan (ref. 15). Geometry, mesh, input data, and the results for the latter problem are given at the end.

- Vertical Fracture Near a Well: The pressure responses for an observation well in a system with a fracture not intersecting, but aligned with a producing and an observation well are compared with the analytic solution of Heber-Cinco et al. (ref. 10).

- Horizontal Fracture: The pressure responses for a horizontal fracture located at the center of an aquifer and intersecting a well in an axisymmetric region are compared with the analytic solution of Gringarten and Ramey (ref. 8).

Field Validation - The code has been tested against problems involving coupling between fluid flow and deformation, specifically laboratory experiments of large rock samples with tension fractures and field tests in shallow fractured formations (ref. 5). High pressure at a wellbore can open up fractures and result in a high injection rate while low pressure at a wellbore during withdrawal can close the fracture and decrease the hydraulic conductivity of flow.

III. General Description

Operating Characteristics - The code is written in FORTRAN IV and is presently being used on the CDC 7600 at Lawrence Berkeley Laboratory. Set-up of the data follows the organization of other finite-element programs at Berkeley. Familiar options of two-dimensional finite-element stress- and strain-analysis and fluid-flow codes are included in this code.

Inputs -

Initial and boundary conditions for stress, pressure, and displacement
Permeability of porous block
Fracture aperture
Porosity of porous block
Compressibility of the fluid
Coupling constant, α, and fluid parameter,
Geometry of domain
Young's modulus and Poisson's ratio for the rock medium
Initial normal stiffness, tangential stiffness, cohesion and angle of friction for the fracture
Fluid density
Fluid viscosity

Outputs - At the end of each time step, the pressure, displacement and the flow flux and the stress components on the elements can be printed. Graphic output of the mesh with the plot of the principal components of stress, and displacement are generated in the program.

Available Documentation - Formal documentation for ROCMAS is to be made available in the near future in the form of a user's manual. Currently available documentation may be found in Ref. 15.

IV. Review of Theory

Equations - In this model, the fluid movement and the solid deformation are coupled. Each point in space, either inside a discrete fracture or within a rock block, has a pressure variable p and a solid displacement vector u_i. Flow is very sensitive to the solid deformation especially within the fractures where the fracture-specific permeability $k = (2b)^2/12$ for parallel-plate laminar flow is used (2b = aperture width).

The mathematical form of the coupling between the fluid flow and the solid displacement can be written as a set of three equations for the pressure-strain, stress-strain and stress-load relations. The first fluid-flow equation is:

$$\frac{1}{M}\frac{\partial p}{\partial t} - \alpha\frac{\partial \varepsilon}{\partial t} = \frac{\partial}{\partial x_i}\frac{k_{ij}}{\mu}\frac{\partial p}{\partial x_j} \qquad (9.10)$$

where α and M are material properties representing the responses of fluid mass content to changes in pressure and changes in volumetric strain $\varepsilon = \varepsilon_{ii}$, and μ is the viscosity.

The volumetric strain depends on the effective-stress field. The fluid pressure, or pore pressure, counteracts normal to the fluid-solid interfaces. The effective stress-strain relation can formally be written in the form of Hooke's law:

$$\tau_{ij} + \alpha\, p\, \delta_{ij} = D_{ijk\ell}\, \varepsilon_{ij} = \sigma_{ij} \tag{9.11}$$

where τ_{ij}, the total stress on the system, is related to σ_{ij}, the effective stress on the solid, through the value of the pore pressure, p.

For isotropic elastic porous rock media, the components of the tensor $D_{ijk\ell}$, in the porous block, can be expressed in terms of two elastic constants, i.e., Young's modulus and Poisson's ratio. For anisotropic, inelastic deformable fractures, the stress-strain relation is very nonlinear. In this model, a bilinear normal stress versus normal displacement relation and a bilinear shear stress versus shear displacement relation are used. The normal and shear stiffness as functions of stresses characterize the fracture behavior. The displacement u_i is simply related to the strain tensor, ε_{ij}, by the component definition:

$$\varepsilon_{ij} = 0.5 \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{9.12}$$

The third equation is Newton's first law of static equilibrium applied to an infinitesimal volume element of the fluid-filled medium:

$$\frac{\partial}{\partial x_i}\, \tau_{ij} + \rho_s\, f_j = 0 \tag{9.13}$$

where ρ_s is the wet bulk density and f_j is the body force. One example of a body force is that force due to gravity. Both the gravity effects on the fluid and rock can be taken into account. Gravitational drainage of fluid can be modeled.

Numerical Approximations - Analysis of a fractured porous medium for coupled stress and fluid flow behavior is made feasible by application of a numerical method. The method used adopts a variational principle (refs. 6, 7).

A finite-element discretization is used to discretize the space domain. The two-dimensional space is decomposed into finite-element quadrilateral domains with four-corner nodes (ref. 17). Each node has the values of three variables: the pressure p and the two components of solid displacement u_i.

Isoparametric bilinear polynomial basis functions are used to interpolate from the nodal values to the space within an element representing the porous rock medium. For a fracture, it is assumed that the aperture is small and fluid flow is along the fracture surfaces. The pressure difference between adjacent nodes across the aperture is negligible, and a one-dimensional element can be used for interpolating between two end-point pressures (ref. 16). For the fracture displacements, it is convenient to take the same spatial (global) coordinates for each pair of points across the small aperture for the four-corner element. However, the relative movements of the surfaces in the direction vertical to the fracture plane and along the fracture are important for the structure analysis. The fracture element in terms of these relative displacements is used (ref. 9). The time discretization scheme used in this model to step from time t to time $t + \Delta t$ is the predictor-corrector scheme. Basically, the solution is first predicted at $t + 0\Delta t$ $(1 \leq 0 \leq 2)$ and then it is corrected by linear interpolation to give the value of the unknown at time $t + \Delta t$. Four-noded isoparametric elements are used in the porous medium with one-dimensional line elements to represent the fractures. Coupling of the pressure field and the mechanical deformation is founded on the extension of Biot's consolidation theory (refs. 2, 3, 4) for porous elastic media to nonlinear fracture behavior.

Probabilistic or Statistical Aspects - None.

Assumptions and Simplifications - The main assumptions and simplifications used in ROCMAS are:

- Two-dimensional flow only is analyzed
- Isothermal conditions exist
- The porous medium exhibits elastic structural behavior
- The fracture-specific permeability $k = (2b)^2/12$ for parallel-plate laminar flow is used in this model
- The fractures exhibit nonlinear structural behavior
- The fracture aperture is small and fluid flow is along the fracture surfaces
- The pressure difference between adjacent nodes across the aperture is negligible.

Structure and Level of Detail - The domain of interest is subdivided into a series of two-dimensional finite elements. This subdivision or discretization appears as a grid over the whole domain. This two-dimensional grid consists of four-corner quadrilateral elements for the porous rock medium and two-node elements for the discrete fractures. The fractures can extend from one boundary to another, intersect each other, or can be isolated in the porous rock medium. An axisymmetric grid can also be used.

Major Dependent Variables - The most important variables describing flow and deformation in a porous medium are:

- pore pressure, p
- solid-displacement components, u_1, u_2.

Applicability, Limitations, Validity and Completeness - The present code treats what is primarily a near-field problem, the coupling between consolidation and fluid flow. However, it does not incorporate thermal effects. The forthcoming version, which is to incorporate heat, is likely to be far more useful.

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APPENDIX A

APPENDIX A
CODES CONSIDERED FOR INCLUSION

In recent years, several groups have attempted to summarize available computation models for analysis of the various processes associated with the field of nuclear waste isolation. The first step in the code selection was to review the summaries of all models described in such references pertaining to repository siting. The majority of the codes reviewed were described in these available summaries. However, due to recent developments, several additional codes that were not in those summaries have also been reviewed. References to the published compilations are given in Table A-1.

In cases where a name was not provided by the references, the model was named after the author or authors. If a code has been so named, it is marked with an asterisk. This procedure is somewhat arbitrary and may lead to some confusion, but it is essential that each code be identifiable for this tabulation.

Only repository siting is considered in this report. The codes were categorized into the following subtypes for the initial screening:

- Saturated Flow
- Unsaturated Flow
- Surface Water Flow and Transport
- Solute Transport without Geochemistry
- Energy (Heat) Transport
- Energy and Solute Transport
- Geochemistry and Solute Transport with Geochemistry
- Geomechanical

The number of codes reviewed in each of these areas may be seen in Table A-2. For the main text of the report, the categories were reorganized by combining all solute transport codes (except those also including heat transport) into a single category and separating out geochemistry codes.

The available codes are listed in Tables A-3 through A-10. It will be noted that this represents only a preliminary categorization. When the codes summarized in the main text were reviewed more carefully, some were found to belong in different categories from those in which they are listed here.

Table A-1. References Used to Identify Available Codes

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Table A-2. Summary of Code Types Reviewed

Code Type	Number of Codes Reviewed
Saturated Flow	34
Unsaturated Flow	12
Surface Water Flow and Transport	18
Solute Transport without Geochemistry	54
Energy Transport	22
Energy and Solute Transport	3
Geochemistry and Solute Transport with Geochemistry	30
Geomechanical	10
Total	183

Table A-3. Saturated Flow Codes

AFPM
BEWTA
COOLEY
COOPET*
ESOPH
FEGWM
FE3DGW
FLOP 1
FLOP 2
FLUMP
FPM
FRICHO*
FRONT-N
GABHYD
GWATER
GWHEAD
LM4
MOLZ*
MTMVMC
NARAS*
PICKENS*
PINBRED*
P1
RCPIGW
RUSHTON*
SHIBASAKI-1
SUPERMOCK
TAYLOR
USGS2D
USGS3D
VTT
V3
WALES (ENG)
WTSHED2

Table A-4. Unsaturated Flow Codes

COLORADO-FD
FEMWATER
FREEZE
FRESURF 1 & 2
FRIVER*
INTERCOMP-GWM
KANSAS-GREEN
NELREI*
PST
REEVES-DUGUID
TRIGAT-HS-1
UNSAT 2

Table A-5. Surface Water Codes

CAFE-1
CAFE-2
DISPER-1
DISPER-2
FETRA and SERATRA
HEC-1
HEC-2
HN-ML
HN-SL
HOTSED
LODIPS
LPGS
MITCAT
SEDONE
SIMFD
SIMFE
WATFLOW
WHITE/GLOYNA

Table A-6. Solute Transport

AHLBAC*
ARNDEJ*
AT123D
AUTOMIG-2A
COFAM
DICKMAN
DPRWGW and DPRWCR
DUGUID-REEVES
DWAGOD*
ECDISP
ECHER
FARMER
FEMWASTE
FRONT
G-PACK
GUREG 1*
GUREG 2*
GUREG 3*
HOLGUI
HYDRO
INEL TRANSPORT I
INTERA HCTM
INTERA 1
ISOQUAD
ISOQUAD 2
KONBRED
MAIN
MIGRAIN
MINUTE
NELSON*
NEWSAM
NRC
OGRE
PATHS
PCP
PERCOL
PINDER
REPFLO
ROBERTSON 1
ROBERTSON 2
SALTRP
SEGOL
SOLTR
STM
TRANSAT
TRANSONE
TRANSTWO
TRENCH
UNFLW
USGS MC
USGS MOC
WATSOL
WHTM
WTQUAL 1

Table A-7. Heat Transport Codes

CCC
CEREBERUS
CHARGR
COATS
FAUST-MERCER
FEG
FRACTURE
GENAESIS
GEOTHER/FAUST-MERCER-3D
HUYAKORN/PINDER
MAGNUM-2D
METERNIQ
SATUNA
SCHAFF
SHAFT79
SPECTROM 55
TEMPER
THOMAS/PIERSON
TORONY1
TRUMP
TRUST
VOSS/PINDER

Table A-8. Heat & Solute Transport Codes

GWTHERM
SHALT
INTERA DWDM/SWIP

Table A-9. Geochemistry Codes and Solute Transport Codes with Geochemistry

ARDISC
AT123D
BIOSSIM
CHAINT
DPCT/SCHWARTZ
EQ3/EQ6
FASTPATH
GARD/GARD2
GETOUT
GEOCHEM
GEOSPHERE
GROVE/GALERKIN
HERMES
LEVINE
MMT
MINEQL
NWFT/DVM
PORFLO
PHREEQE
RAMM
REFQS
SOLMNEQ
SWIFT
TEHM
TRANS
UTM
VCHFLD
WASTE/NUTRAN
WATEQ/WATEQF
WIGKNI*

Table A-10. Geomechanical Codes

CONDAM
DNET
GLM
HART
PORFRC2
ROCMAS
SHIBASAKI-2
SHIBASAKI-3
TERZAGI
TRUST

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This report is the first in a series of reports that will provide critical reviews and summaries of computer programs that can be used to analyze the potential performance of a high-level radioactive waste repository. The computer programs identified address the following phenomena: saturated and unsaturated subsurface flow, heat transport, solute transport, surface water runoff, geomechanical interactions, and geochemical interactions. The report identifies 183 computer programs that can be used to analyze a repository site and provides a summary description of 31 computer programs. The summary descriptions can be used: to assist in code evaluation, to facilitate code comparison, to determine applicability of codes to specific problems, to identify code deficiencies, and to provide a screening mechanism for code selection.

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