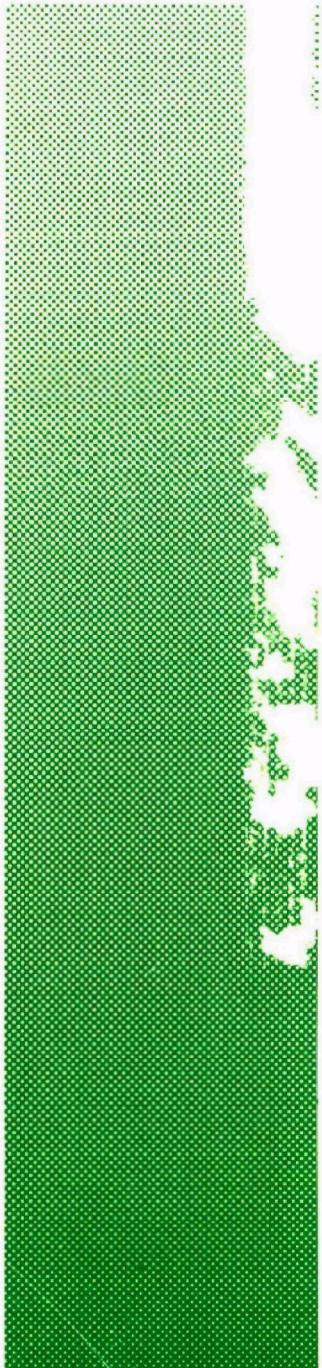
Modeling and Low-Level Waste Management: An Interagency Workshop

December 1-4, 1980

Denver, Colorado



Sponsored by

U.S. Department of Energy

U.S. Environmental Protection Agency

U.S. Geological Survey

U.S. Nuclear Regulatory Commission

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A17 Microfiche A01

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Modeling and Low-Level Waste Management: An Interagency Workshop

December 1-4, 1980
Denver, Colorado

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Workshop sponsored jointly by U.S. Environmental Protection Agency, U.S. Nuclear Regulatory Commission, U.S. Geological Survey, and the Oak Ridge Operations Low-Level Radioactive Waste Management Program, U.S. Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation.

Date Published: June 1981

Preface

This workshop was organized by the Interagency Low-Level Waste Modeling Committee and was held December 1-4, 1980 in Denver, Colorado. Committee membership is listed on the title page. Each of the four federal agencies represented on the committee contributed equal funding to support the meeting.

The paramount objective was to foster cooperation between the agencies having various responsibilities and involvements in modeling for low-level waste applications. Another aim of the workshop was to begin a dialogue between model users, such as regulators and assessors, and modelers. These Proceedings are testimony that progress has been made toward attainment of these goals.

The meeting had three distinct sessions. First, each agency presented its point of view concerning modeling and the need for models in low-level radioactive waste applications. Second, a larger group of more technical papers was presented by persons actively involved in model development or applications. Each of these papers came from one of the sponsoring agencies or from an agency contractor. Last, four workshops—two running concurrently—were held to attempt to reach a consensus among participants regarding numerous waste modeling topics. Each of the three sections is identified in the Contents.

We are grateful to many people for their assistance in organizing the meeting and compiling the Proceedings: speakers and authors who promptly delivered their manuscripts; workshop chairmen and secretaries who recorded and summarized their sessions; Bonnie Reesor of the ORNL Conference Office; and particularly Thelma Patton and Brenda Baber of the ORNL Low-Level Waste Management Programs Office. Thanks.

Craig A. Little
Secretary for Interagency Low-Level
Waste Modeling Committee

June 1981

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USDOE NEEDS IN MODELING FOR LOW-LEVEL RADIOACTIVE WASTE MANAGEMENT

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Greetings from John Peel who is Manager of the National Low-Level Waste Management Program (NLLWMP) for the Department of Energy Idaho Operations. Speaking for him and as Associate Program Manager of the NLLWMP for Technology Development for Oak Ridge Operations, we will give you this Program's perspective of the DOE's requirements for modeling in Low-Level Radioactive Waste Management.

On the agenda, this presentation is entitled, "USDOE Needs in Modeling for Low-Level Waste Management." At the outset, we want to emphasize that the Department of Energy does not need additional models as entities. We do need reliable and credible tools for decision making which involve identification, selection, adaptation, and implementation of existing models. This is an important distinction and is the basis for the Low-Level Waste Management Program's efforts in environmental modeling. Recently, the Program issued a strategy document which endorses states being allowed to assume and implement their responsibilities for managing their respective low-level wastes; it identifies areas of assistance that federal agencies can provide to states. In summary, the states must decide upon a course of action regarding siting and selection of disposal sites; making that decision often requires and is expected to use environmental models as decision-making tools.

We are not being trite when we emphasize that an environmental model is only a tool that can be used in a decision making process and should not be used as a replacement for management judgement. The value of a model is to focus complex technical considerations to provide management with the ability to examine various options, compare impacts, and to explore the mitigative effects of alternatives. If and when it becomes necessary, models are used to predict events and to aid in resolving the "What if?" questions. The reliability for prediction is, of course, a function of the model itself, but as importantly, the accuracy of the input data. Because of the inherent inaccuracies and uncertainties of data, or simplifying assumptions used when data do not exist, the reliability of model prediction will always be subject to question. For this reason, decision making cannot and should not be based solely on model prediction.

In July, many of you attended a meeting on Low-Level Waste Modeling held in Bethesda, Maryland. At that meeting, several key issues common to all modeling groups were identified. Tonight, let

us examine some conclusions reached at that meeting and how the Program intends to proceed in its modeling efforts. We will also present some issues which we believe can only be resolved through interagency cooperation.

An important conclusion at our July meeting was that many models lack credibility. Consequently, a "Credibility Gap" does exist. This is partly due to ineffective use of models; but, as importantly, it is due to a lack of understanding by model developers of what is required for decision making. Are models really telling us what we need to know? Models are used to predict, but results are often presented as absolute numbers. When looking at those numbers, how often have you seen model results that attempt questionable accuracy and predict one "FEMTO-REM" per billion population? These numbers do not deal with a real world situation; and, based on cause-effect relationships, such a degree of precision is neither necessary nor desirable.

Clearly, there is a need for model developers to state what their models can do and provide some bounds or limitations on model results. Concurrently, the user must be educated concerning the real function of that model and not attempt to push it beyond the limits of credibility. This brings up another point concerning credibility. How often have we seen "worst-case analysis" end up as "absolute truth"? Decision making is an interactive process between government and public. A report analyzing some worst case scenario may be so prohibitive that reasonable alternatives may be ignored. As our colleague Jerry Cohen says, "Give me a worst case and I'll develop yet a worse one." We must reemphasize the use of engineering and management judgement in defining model scenarios. Our principal short term goal is to provide a siting model by September 1981. Until this task is completed, the program will not be able to identify and support other areas of model development work. We have neither the time nor the funds to conduct extensive new model development, and we do not believe that such effort and expense is necessary since many adequate models already exist.

The siting model is needed by decision makers to examine the adequacy of a site, explore various alternatives, and develop preliminary operating and design criteria.

The basic guidance for our model development has been that the model should:

1. Estimate health effects and maximum dose to any individual for the population at risk;

2. Estimate the health effects with reasonable accuracy;

3. Estimate the health effects within a reasonable cost of computer execution;

4. Be as simple as possible while giving adequate detail for standards development; and

5. Be comprised from existing sub-models; when adequate sub-models are available, thereby reducing development time and costs.

Our approach to model development has been to:

1. Review existing models;

2. Select viable models;

3. Utilize viable sub-models from selected models; and

4. Fill in gaps with new sub-models.

Our consideration and treatment of models include:

1. Verification and validation

   The credibility of a model is dependent upon its ability to simulate and predict. A verified model reasonably simulates physical transports and pathways; whereas, a validated model predicts (within limitations) actual transport of a substance. There are many models that cannot be validated because of simplifying assumptions used in their development. But, any model to be used in decision making must, as a minimum, provide a reasonable simulation of the real world. The majority of our laboratory and field efforts will be directed toward validation and verification.

2. Improved characterization

   Unreliable or inadequate data will always reduce the credibility of model results. Field measurements and uniform site characterization procedures are necessary to improve input data.

3. Bounding the credibility of model results

   Sensitivity analyses, error bars, and probabilities are important. Errors in input data should be propagated through the model to provide estimates of result error. Sensitivity analyses identify limitations of model boundary conditions. Analysis of probability allows the user to identify the dominant pathways and events. All of these serve to bound the credibility of the results and provide the user with an understanding of the model's limitations in decision making.

At this time, let us turn our attention to a discussion of criteria. A model should be used to determine how effectively a site will meet criteria. At the present time, we do not have recognized and approved criteria for reference of implementation. The federal agencies must come to an agreement on what we are expecting models to provide; until we have such criteria, it may be pointless to continue modeling.

The most basic criteria should be expressed in terms of the maximum allowable doses to the public from routine and accidental releases. In determining these criteria, we must take into consideration the economic impact on industry and the principles of as low as reasonably achievable (ALARA).

The 500 mrem maximum individual exposure limit is based on sound scientific evidence and reasoning. It is a regulation and industry standard. However, do we select and operate sites based solely on the 500 mrem limit or do we establish some lower limit? If we establish a lower limit, is it scientifically defensible, and can we justify the economic impact on industry? For purposes of discussion, let us examine the following "straw man" criteria:

1. The maximum allowable dose from any accident or non-routine release is 500 mrem under normal conditions.

2. The physical properties of that site should not permit exposure of individuals to more than 50 mrem under normal conditions. This does not take into account any properties for waste form or special retardation barriers but is based solely on waste inventory and the site characteristics.

3. The dose from a release event should be inversely proportional to the probability of the event. This, of course, means the higher the probability, the lower the dose.

4. Sites are to be selected, designed, and operated so that during operational periods the maximum dose will not exceed 500 mrem; for the 25 years of post-operational monitoring, the maximum dose does not exceed 100 mrem; and after 25 years the maximum dose does not exceed 50 mrem. This last "straw man" criteria is our obligation not to pass on to future generations a burden for maintaining these sites.

One way for a decision maker to determine if his site meets these "straw-man" criteria is through the use of a model. Based upon our experience, it would seem that such criteria would not only be easy to meet but also difficult to violate under any reasonable management system. Given the guidelines we have suggested, it might be that sufficient modeling capabilities already exist to provide reasonable assurance of compliance.

The following are a few major items we believe can only be resolved through the effective interaction of the federal agencies:

1. Reference sets of source term and dose conversion factors

   There is a need to establish a set of reference source terms to describe a low-level radioactive waste site. One of the major complaints of model users and developers is that too much time and effort is spent in developing source terms, and there is no guarantee that those terms will be considered reasonable. There already exist several excellent detailed source term documents; all that is required is for the interagency group to agree on terms and compile these into a single reference document.

2. Standard documentation format

   A model to be transferred must be in a form easily understandable to the user. There is a need to develop procedures and formats for documenting and transferring models from developers to users.

3. Standard site characterization procedures

   Collection of data for the characterization of a site are not uniform procedures and result in large variances in data. A set of reference characterization procedures should be developed to identify data to be collected and acceptable collection methods.

4. Validation experiments

   This was an idea proposed at our July meeting. In essence, we would develop experiments that would test various scale model shallow land disposal facilities to points of failure. The data obtained would be used to define the conservativeness of our models.

5. Reference validation data sets

   Data from field tests should be developed into a reference document which would allow model users to test their models against real world data.

6. Model categorization system

   Model users often have little to guide them in selecting a model. By providing a categorization system, models would be grouped according to function, application, and boundary condition. This categorization system should be developed concurrently with the model documentation procedures.

In conclusion, we believe that by working together with common objectives the several agencies and supporting organizations can successfully find adequate tools and use them to make appropriate decisions for managing the Nation's low-level radioactive waste.

MODELING AND ANALYSES TO SUPPORT EPA's LOW-LEVEL RADIOACTIVE WASTE STANDARDS

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ABSTRACT

EPA is developing a generally applicable standard for the management and disposal of LLW as part of the U.S. National Radioactive Waste Management Program. It will issue a proposed standard in September, 1981, and a final standard in early 1984. EPA will use predetermined models to estimate the health risks and costs/benefits from disposing of LLW by a number of land and sea disposal alternatives. These estimates will be used to support EPA's decision on the proposed standard and for the supporting EIS and Regulatory Analysis. This paper describes why EPA is using a generic "systems" approach to modeling the impact of LLW disposal, the types of disposal alternatives which will be evaluated, its approach to cost/benefit analysis, the current status of model development, general input data requirements for the model, and a general schedule for development of the models and the standard.

THE NEED FOR A STANDARD --- AND MODELING

Before 1975, there was no demonstrated need for an environmental standard for the disposal of low-level radioactive waste (LLW) because it was believed that there would be no release of radioactive from the disposal sites.(1) Since then, studies at the Maxey Flats (KY), West Valley (NY), and Oak Ridge (TN) disposal sites have shown that unplanned releases to the uncontrolled environment can occur if LLW are not properly disposed and that the impact of these releases could be substantial. For example, more than 24.6 million liters of radioactive leachate containing appreciable concentrations of H-3, Co-60, Sr-90, Cs-137, Pu-238, and Pu-239/240 have been pumped from the trenches at Maxey Flats and treated.(2) Pumping operations are continuing. If stopped, these radioactive leachates would be released by overflow directly at land surface or to the groundwater. The experience at West Valley has been similar.(3)

The public has become increasingly concerned about the safe disposal of all radioactive wastes including LLW. Generators of LLW have become very concerned about the lack of adequate disposal space

in the future since three of six operating commercial LLW disposal facilities have closed. State regulators have become concerned about the quality and the quantity of LLW being shipped to the disposal sites in their states. These occurances established the need for EPA to act pursuant to its charge to identify radiation hazards to the general environment and to set generally applicable environmental standards where needed.(4,5) On February 12, 1980, the President directed EPA to develop the necessary radioactive waste standards on an accelerated basis.(6)

Consequently, EPA is developing a generally applicable environmental standard for the management and disposal of LLW. It has guidance on how to develop this standard from a number of sources. These include NEPA (7), EPA's "Improving Government Regulations" (8), BEIR II (9), "Decision Making in EPA" (10), and ICRP-26 (11). This guidance, which clearly establishes EPA's needs for modeling and models, has been summarized quite well in EPA's proposed "Criteria for Radioactive Wastes" (12) as follows,

"...Radiation protection requirements for radioactive wastes should be based primarily on an assessment of risk to individuals and populations; such assessments should be based on predetermined models..." and

"...Any risks due to radioactive waste management or disposal activities should be deemed unacceptable unless it has been justified that the further reduction in risk that could be achieved by more complete isolation is impracticable on the basis of technical and social considerationd..."

Before going on to discuss EPA's general modeling needs, the role of modeling in EPA's standards development process should be put into perspective. MODELING IS ONLY A TOOL! Developing and setting environmental standards is less than an exact science. In most cases, arrival at the standard involves a combination of public acceptance, political accord, good judgment stemming from long experience in public health protection, and expert technical judgement. The models will <u>support</u> our judgement and standard. The results from our modeling efforts will not be <u>the basis</u> for EPA's standard.

EPA'S APPROACH - A GENERIC "SYSTEMS" APPROACH

The primary purpose of EPA's modeling efforts is to assess the potential impacts from managing and disposing of LLW by a number of realistic alternatives. This includes estimating the potential releases to the environment, doses, health risks, and costs.

A number of factors have influenced EPA's approach to doing this. These factors, which include EPA's authorizing legislation and mandates, the character of the wastes, themselves, and the realistic means by which they may be managed or disposed, are discussed briefly below.

The guidance given to EPA for developing the standard is broad, general, and sometimes contradictory. The environment should not be degraded.(7) We should assess the impact of all reasonable alternatives.(8) Even the smallest amount of radiation is harmful.(9) The risk should be reduced as low as reasonably achievable (ALARA) but we should take social and economic factors into account.(9,11,12)

The radioactive wastes for which this standard is being developed are an extremely heterogeneous group of wastes. They include all wastes which have been categorized as "low-level" radioactive wastes and, in addition, those transuranic-contaminated wastes (TRU) which do not fall under the High-Level Radioactive Waste (HLW) Standard.(13) The term "low-level" does not adequately reflect the potential hazard of wastes currently classified as LLW. LLW are, in fact, a large diverse class of wastes in which some types may contain tens of thousands of curies per cubic meter (14,15) and remain radioactive for millions of years. Other LLW may contain only traces of radioactive material. They may be solid, mushy, liquid, or gaseous; may range from insoluble to completely soluble; and may be animal, vegetable, or mineral.

Disposal in the ground or in the ocean are the disposal methods which are most readily available at this time. Any land or ocean disposal facility is a complex "system" which includes the waste, the site geology, hydrology or oceanography, and meteorology, the emplacement method, site engineering, and all of the pathways from it --- and the performance of the system will change if changes are made to any of its parts. Analysis of a single pathway would not provide an adequate analysis of the impact of a "disposal system." Thus, the disposal facility and the wastes in it must be regarded as a disposal system and analyzed as a whole if we are to assess its overall impact.

Because of the above factors, our model(s) will be used to evaluate the effectiveness of each disposal alternative using a systems approach --- to examine each alternative as a disposal system and to compare it with alternative disposal systems. Sufficient detail will be included in the models to permit evaluation of the effectiveness of proposed changes in the system design for improving the retention capability of the disposal system

(i.e., change in waste form or packaging, engineering barrier, etc.). Changes in the design of the disposal system may also affect the cost of disposal. These costs will be assessed or modeled separately.

There are a number of land and sea disposal methods which are suitable for the disposal of some types of LLW. However, no one disposal method is suitable for all types of LLW. Therefore, the model(s) should be applicable to a variety of disposal methods, types of wastes, and hydrogeological settings; the results of which should be useful in comparing the potential impacts and costs of the different disposal alternatives. Thus, it is also clear that a generic systems model(s) is needed.

The natural characteristics of a disposal site or "disposal system" (i.e., geology, hydrology, and meteorology) are determined and relatively fixed once a site is selected. Normally, they can be changed by selecting another site. However, emplacing wastes in the site, the interaction of the wastes with the site, and engineering changes to the site can significantly alter the functioning of the hydrogeologic portion of the "disposal system" and directly affect its performance. The wastes, their form, the method of their emplacement, and site engineering also affect the performance of the "disposal system" but are mainly determined by man. The point being made is --- the natural characteristics of the "disposal system" are mainly determined in the site selection process; man can control the performance and costs of the rest of the system.

TYPES OF ENVIRONMENTAL ASSESSMENT MODELS

We have reviewed a number of alternative methods for disposing of LLW to identify those which could be implemented quickly without delay for technical hardware or development. So far, we have identified eight land and two ocean disposal methods which could be used for the disposal of one or more types of LLW. Our review has shown, however, that not one of these methods is suitable for the disposal of all types of LLW.

In five land disposal methods, the wastes would generally be disposed of at or near land surface and generally not below 50 meters depth. These shallow land disposal (SLD) methods include engineered surface storage (SLD-SS), sanitary landfill (SLD-LF), shallow land disposal as presently practiced (SLD-P), improved shallow land disposal (SLS-I), and intermediate depth disposal (SLD-I). In three land disposal methods, the wastes would generally be disposed of at depths greater than 50 meters. The deep land disposal (DLD) methods include deep geological disposal in a mined cavity (DLD-MC), hydrofracturing (DLD-HF), and deep-well injection (DLD-DWI). The two ocean disposal methods include disposal on the

sea floor (OD-OSF) and beneath the sea floor (OD-BSF). We are, therefore, developing environmental assessment models for shallow land disposal (SLD), deep land disposal (DLD), and ocean disposal (OD).

The SLD assessment model will be used to analyze the potential health risk from disposing of LLW at or near land surface to a depth of 50 meters but generally above the water table. Experience has shown that near surface geology, hydrology, and meteorology affect the performance and retention capability of a SLD site very much. Therefore, the SLD model is being designed with sufficient flexibility to cover at least three types of wide-spread hydrogeologic/climatic settings which we believe will cover the most sensitive parameters that affect radionuclide retention and site performance. These settings include: (1) an arid zone site for which no particular regard is given to the permeability of the disposal medium (because of a lack of water as a driving force); (2) a humid zone site with a low-permeability disposal medium (which would fill like a "bathtub" in the event the trench cap leaked); and (3) a humid zone site with a moderately permeable disposal medium (which would allow water infiltrating through the trench cap to leak out the bottom of the trench like a "sieve").

Additional settings will be developed as necessary by altering in the input parameters. The water pathways would certainly be less important for conventional SLD and improved SLD in the arid climates, whereas, all of the pathways would be important for these methods in the two humid climate scenarios. For intermediate depth SLD (10-18m deep), the groundwater pathway would be considered most important.

The DLD assessment model will closely parallel the SLD assessment model in design, pathways, etc. However, it will basically be used to analyze the impact of disposing of LLW at depths below 50 meters and generally below the water table, although there are some areas in the western United States where water tables are as deep as 700 meters. Near surface hydrogeology and meteor ology normally will not have much affect on the performance of the DLD alternatives. More emphasis will be given to hydrodynamics and groundwater transport.

There is not sufficient information on the ocean disposal assessment model to discuss it at this time.

BENEFIT/COST MODELING

The benefit/cost analysis program to support the LLW waste standard will be different and more extensive than the one conducted

for the HLW standard. To begin with, we have extensive experience and impact and cost data from operating SLD facilities. These data can be used to develop a base case against which other disposal methods can be compared. For HLW, there was no such experience or data. There are also at least ten alternatives for disposing of LLW for which the benefits and costs can realistically be estimated and compared. No comparison was made for HLW. Finally, the length of time which LLW must be retained is generally much less than for HLW; in most cases, only several hundred years or less rather than thousands of years. Thus, the period of analysis can be much shorter for LLW.

The benefit gained in waste disposal, as used herein, is the reduction in health effects gained from taking a control action. The greater the reduction in health effects, the greater is the benefit. The benefits, or reduction in health effects, which may be gained from each disposal alternative will be calculated using one of the SLD, DLD, or OD assessment models discussed earlier. To help the user, the benefits will be expressed, so far as possible, in several forms including radionuclides released to the environment and doses, health effects and health risks to individuals and populations.

On the cost side of the analysis, one, and possibly two, analyses will be made. The projected direct costs for controlling or disposing of a unit of waste, whether it be in specific activity or unit volume, will be estimated for each disposal alternative considered. These costs will be useful for the tradiational "cost-effectiveness" types of analysis. They will also furnish guidance on how much is being spent on the control of LLW. A model(s) or method(s) will be developed to calculate and compare these direct costs for the different disposal methods.

A second, broader type of economic analysis may be required, depending upon whether EPA internal triggering criteria relating to total dollars for costs of compliance, increases in energy consumption, etc., are met.(8) The purpose of these economic analyses would be to fully identify, on a national basis, the overall benefits and costs of the regulations; not just the direct costs. They would include preparation of a profile of the affected sectors of the economy including producers, consumers, and industry. The following impacts would be analyzed: price effects; production effects; industry growth; profitability and capital availability effects; employment effects; balance of trade effects; and energy effects.

CURRENT STATUS OF MODEL DEVELOPMENT PROGRAM

As noted earlier, our general modeling program is directed at making realistic technical analyses of the health risks and costs of disposing of LLW by a number of practical disposal alternatives. The major steps and flow of achieving this goal includes: defining our modeling needs and approach; developing the models; compiling data on the wastes, disposal alternatives and actual disposal sites to use in the models; and conducting the analyses.

Definition of our modeling needs and approaches to environmental assessment modeling is being done in-house. The concept and design of our SLD model is complete.(16) Design is in progress on our DLD and cost models. Design of the OD model has not begun yet.

Specific guidance for development of the infiltration, leaching, and groundwater transport submodels for the main SLD assessment model release was developed in-house by Dr. C. Y. Hung.(16,17,18,19). The submodels for the atmospheric and terrestrial pathways submodels and dose and health risk which will be used in the SLD model are models which were or are being developed for EPA for use in the Clean Air Act.(20,21) They were developed by Oak Ridge National Laboratory (ORNL). ORNL is currently developing our SLD assessment model under an interagency agreement with DOE. This includes development of several additional submodels and, as necessary, modifying and coding all of the submodels into an overall main assessment model.

The overall design and submodels of the DLD assessment model will closely parallel the SLD model. The major difference is that the DLD model will be used to analyze the impact of disposing of LLW at depths below 50 meters and generally below the water table. The DLD model will probably include the modification and combination of submodels from our HLW model and the SLD model currently being developed. However, the dose/health risk model used will be the one from the SLD model, which is different from the one currently used in our HLW model. Work on the DLD model has not begun yet, nor has work on the cost model.

Disposal of LLW on and beneath the ocean floor, which includes two of ten disposal options currently considered practical, is regulated under different authorities than land disposal. The ocean disposal program is moving at a different pace than the LLW program. At present, evaluations of former ocean disposal sites, development of siting criteria, and evaluations of ocean disposal technology are under way. However, development of an environmental assessment model for ocean disposal appears to be several years in the future.

INPUT DATA FOR THE MODELS

With an estimated 20 million dollars or more per year being spent by other Federal Agencies on research and development for LLW management, we believe that most of the data needed to support EPA's models is either already available or is being collected by others. Therefore, most of EPA's efforts will be directed at collecting, collating and critically evaluating data from others. We are presently carefully reviewing the information available on radioactive and hazardous waste-related projects funded by other Offices within EPA, other Federal agencies, the States, and industry, to facilitate rapid collection of the needed data. Gaps in our data needs will be filled as necessary.

Field data will be collected from three existing LLW disposal sites to provide actual or, at least, realistic data for input into the SLD assessment model and for making the cost/risk analysis for disposing of LLW by this method. The sites are Barnwell (SC), West Valley (NY), and Beatty (NV) which represent the three general regional hydrogeological and climatic settings we intend to model.

Two categories of site data will be collected; one from existing data, including published and unpublished data, and the other from field observations. Existing data will be used whenever possible. ORNL is currently preparing a list of data needs for the SLD model and is compiling some of the existing data. Collection of additional data to fill in the gaps between the model data needs and the existing site data will start shortly.

We currently have an in-house project for compiling and evaluating information on waste characteristics and on improved methods for treating, packaging, and managing LLW. This information will be used to estimate the potential costs and reductions in health effects which can be achieved through waste management alternatives which already exist. Information is being collected on: the character and quantities of primary wastes being produced by typical waste generating facilities before treatment and packaging; what kinds of segregation and elimlination of wastes may be done within each facility; the treatment, volume reduction, solidification, and packaging options that are available for the primary wastes and the characteristics and quantities of the resulting wastes; the hazard potential of the various wastes; and projections of future wastes based on several optimum management and treatment modes.

We will soon begin to collect information and develop the general characteristics of the natural (geological), engineering, and institutional barriers which are currently being used, or could

be used in the near future to retain LLW when disposed of by shallow land disposal and other selected land disposal alternatives. The types of land disposal methods to be considered was discussed earlier. Information to be collected includes; technical and cost data on SLD as presently practiced, improved SLD, and the other land disposal alternatives; site selection criteria for all land disposal alternatives; and post-operational controls for all land disposal alternatives.

TIMING FOR DEVELOPMENT OF LLW MODELS AND STANDARD

The schedule for development of the LLW standard, development of the models, technical, environmental and cost assessments, and collection of data to support the assessments is shown in Figure 1.

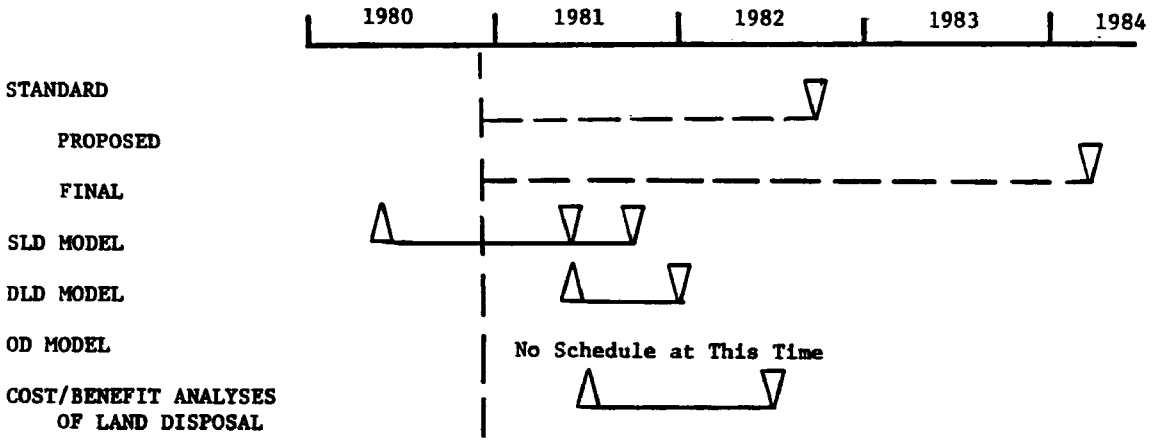

Figure 1. General schedule for the development of EPA's LLW assessment models, analysis of the risks, costs and benefits of different disposal alternatives, and development of the LLW standard.

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MODELING IN LOW-LEVEL RADIOACTIVE WASTE MANAGEMENT FROM THE U.S. GEOLOGICAL SURVEY PERSPECTIVE*

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ABSTRACT

The United States Geological Survey (USGS) is a long-standing proponent of using models as tools in geohydrologic investigations. These models vary from maps and core samples to elaborate digital computer algorithms, depending on the needed application and resources available. Being a non-regulatory scientific agency, the USGS uses models primarily for: improving modeling technology, testing hypotheses, management of water resources, providing technical advice to other agencies, parameter sensitivity analysis, and determination of parameter values (inverse problems). At low-level radioactive waste disposal sites, we are most interested in developing better capabilities for understanding the groundwater flow regime within and away from burial trenches, geochemical factors affecting nuclide concentration and mobility in groundwater, and the effects that various changes in the geohydrologic conditions have on groundwater flow and nuclide migration. Although the Geological Survey has modeling capabilities in a variety of complex problems, significant deficiencies and limitations remain in certain areas, such as fracture flow conditions and solute transport in the unsaturated zone. However, even more serious are the deficiencies in measuring or estimating adequate input data for models and verification of model utility on real problems. Flow and transport models are being used by the USGS in several low-level disposal site studies, with varying degrees of success.

INTRODUCTION

A model generally means a simulator of a thing or process that cannot easily be observed directly. This broad definition is applicable to use of the term in the U.S. Geological Survey (USGS) and in this presentation. Everyone uses models, whether they be analogue, mathematical, or conceptual. Our favorite photographs of people and scenes are

*This paper is prepared for inclusion in the program of the Interagency Workshop on Modeling and Low-Level Waste Management, December 1-4, 1980, in Denver, Colorado, sponsored by the DOE-NRC-EPA-USGS Interagency Low-Level Radioactive Waste Committee.

simplified models of more illusive and complex real-world conditions. What driver hasn't used a road map as a scale model of the real highway system? (That example alone quickly teaches us lessons in the problems of model inaccuracies.) Nearly all of us use our car radio or home stereo to simulate our favorite live-music performances.

Scientific models are often thought of as mysterious, electro-mathematical devices fully understood by no one and worthy of considerable distrust. However, the most commonly and confidently used models in science and technology are similar to those used by most everyone else — photographs, drawings, diagrams, and simple equations. The types of models chosen, and the ways in which they are used, simply depend on the desired output and available resources. Types and applications of models used by the USGS are those appropriate to the Agency's mission and its resources. The same is generally true of other agencies and organizations. Before elaborating on the USGS's use of models in low-level waste management technology, it would seem appropriate first to describe the mission and philosophy of the Survey as it relates to radioactive waste disposal. This should help clarify the differences in modeling philosophies and approaches between the Survey and various other Federal or State agencies. These differences often appear confusing, conflicting, or even contradictory, though in reality they are usually complimentary.

WHAT IS THE USGS?

The Geological Survey is an old-line Federal agency established by an act of Congress in 1879 and charged with the responsibility for "classification of the public lands and examination of geological structure, mineral resources, and products of the national domain." It is the Nation's principal source of information about its physical resources — the configuration and character of the land surface; the composition and structure of the underlying rocks; the quantity, extent, and distribution of water and mineral resources. In contrast to many agencies, the Survey's mission has changed very little in more than 100 years; it remains principally a scientific research and fact-finding agency, rather than an action or regulatory organization.

Most of the USGS activities in waste disposal stem from its responsibility to provide data on surface and groundwater quality essential to the development and conservation of water resources. Fundamental in this mission is the development of appropriate technology and tools to better assess physical and chemical behavior of hydrologic systems and their response to stress.

The Water Resources Division of the Survey has a line item in its appropriation to conduct investigations and research aimed at establishing a technical basis upon which earth science criteria can be developed, tested, and enforced by other agencies for the selecting and operating of low-level waste disposal sites. This program includes several field

investigations of existing commercial disposal sites and more fundamental research into such fields as groundwater geochemistry and modeling techniques.

As the Federal Government's principal earth-science research agency, a fundamental part of the USGS role is that of technical advisor and consultant to other Federal agencies and states. The Survey is often mandated by the President or Congress to provide specific technical services to Federal and state programs. A recent example is our Presidentially specified participation in the National high-level waste management program. Our role as technical consultant to other agencies includes critical review of proposed regulations and criteria, investigations of Federal waste disposal sites, review of proposed and ongoing programs, cooperative investigation at the requests of states, and other related investigations, generally of nonregulatory nature. It is generally the policy of the USGS to avoid specific disposal site selection and characterization studies, preferring instead to provide technical advice and tools for other groups to conduct such investigations properly.

Specific states, for example, have come to us for help in searching for a low-level waste burial site. Rather than suggest specific sites, we recommend approaches based on our knowledge of positive and negative factors that appear important in site performance. In addition, we offer any regional, areal, or local data which we have gathered that could be pertinent to their considerations. Our role is restricted solely to earth science considerations, whereas other agencies such as EPA and NRC must consider much broader social, political, legal, and technical issues. Therein lies the fundamental difference between USGS and the other, more action and regulation-orientated, agencies.

MODELING APPLICATIONS IN THE USGS

The Geological Survey has long held a keen interest in development and application of models as tools for quantitative analysis of complex hydrologic problems. Models have always been regarded by the Survey as means, rather than ends, to problem solving. The principal use of models is to aid in gaining a more quantitative understanding of complex hydrologic systems involving many interdependent physical and chemical processes and boundary conditions. Waste disposal and contamination problems represent some of the most complex problems investigated by the Survey. For many of these problems, modeling is the only means we have of examining all major components of a system together.

Another key application of models is to test and evaluate our concepts of system dynamics. Interpretations of field conditions generally must be based on very limited field data. The integrated picture developed from a few point-observations can often turn out like the blind men and the elephant. If one set of data indicates the elephant is like a snake, a model can be constructed to simulate the snake-like attributes. If the model is good, it would soon indicate that a snake's

characteristics and behavior are different from those of the elephant's trunk, suggesting that our initial impression was wrong and that more data are required. Eventually we might obtain data from enough parts of the elephant to construct a model that confirms our blind interpretation of the beast.

Models have been used extensively to help interpret hydrology and decipher performance of existing low-level radioactive waste burial sites. These sites represent long-term complex experiments whose results we are currently observing and recording. The unknowns in these experiments are the experimental conditions. The challenge then, is to determine the experimental conditions that produced the results currently observable. Models are one of the few tools that can allow us to test various combinations of conjectured conditions. One of the most important outputs of this type of modeling is a sensitivity analysis — a ranking of processes and parameters according to the magnitude of their influence on the result of interest (perhaps the concentration distribution of a particular nuclide). These results then serve as guidelines for more detailed studies. Thus, the model output (combined with all of our other tools) can be invaluable in selecting which segments of a system deserve more attention.

Our philosophy is to engage the use of modeling early in any complex study as a feedback tool — repeatedly adjusting the model, in an iterative procedure, as new information is gathered, accompanied by corresponding adjustments in data-gathering and testing priorities, according to modeling results. This application of modeling is immensely helpful in establishing earth-science guidelines for disposal site selection and operation.

Another example of USGS model employment is in resource and problem management. We are often requested to assess impacts of various development options on an aquifer so that a management agency can make sound development decisions. This may involve geochemical and hydraulic impacts of a potentially degrading activity such as a waste disposal facility; or it could involve assessment of various remedial approaches to a contamination problem.

Finally, USGS modeling capabilities can be used as an independent test and verification of modeling results of other agencies used for judging the conformance of a particular site to regulatory criteria. This can be done directly or by providing the appropriate models to other agencies for their use. We view this as one of our most important roles — developing more accurate, more versatile, and more efficient models for use by other government organizations. We maintain several research projects dedicated to advancing model technology and teach courses on modeling open to some non-USGS personnel.

WHAT KIND OF MODELS DOES THE USGS USE?

As mentioned previously, the Geological Survey uses many types of models, ranging from core samples to elaborate room-sized physical models. Although the types of models generally depend on the need and available resources, USGS modeling can be classified into two general approaches.

The first approach is to use a small sample or portion of the real field system to represent the total system. A core sample is an example. In some studies, a core sample might be used for measuring hydraulic properties which might then be extrapolated to represent those properties over a much larger field area. Water samples similarly are often used as models to represent chemical characteristics of a larger zone of an aquifer. These models generally have very limited use and, in fact, have been commonly misused. Hydraulic conductivity measurements on core samples, for instance, are often orders of magnitude different from average areal conductivities in many formations.

The second approach is use of models that simulate the entire system of interest, generally in some simplified way. One of the first, and still the most commonly used model of this type in groundwater hydrology, is Darcy's Law:

$$q = -K \frac{\delta h}{\delta x}$$

where

q is the water flux rate, L/T

K = hydraulic conductivity, L/T

$\frac{\delta h}{\delta x}$ = hydraulic head gradient, dimensionless

This empirically based model is the basis for nearly all other more sophisticated groundwater flow and solute transport models. One of the more elaborate of these (but still simple) is the Theis equation (Theis, 1935), which is perhaps the most widely used model in the world for interpreting the hydraulic characteristics of aquifers. Although very few actual field conditions meet the strict qualifying conditions for application of the Theis equation, it has nonetheless enjoyed widespread success as an approximation.

Models receiving most attention in recent years are, of course, ones which approximate solutions to complex partial differential equations of flow, solute, and energy transport. These models range from elaborate physical and electrical analogues to ingenious mathematical schemes to solve huge matrices of simultaneous equation. These mathematical approaches include a variety of finite difference schemes, such as iterative-alternating-direction-implicit procedure, and various finite

element algorithms such as the Galerkin procedure. All of these methods and a number of others have advantages and disadvantages for different applications. It is not the purpose of this paper to describe or compare these models. Anderson (1979) made an excellent review of model use for simulating contaminant movement in groundwater.

One of the few examples of the development of application and verification of a numerical model to a low-level waste problem was by Robertson (1974). In that case, the field-observed distributions of chloride, tritium, and strontium-90 in a large aquifer were successfully simulated by a two-dimension transient flow and transport model which included effects of dispersion, radioactive decay, and cation exchange. Figure 1 indicates one of the results of that modeling effort for tritium.

We have recently attempted to model groundwater flow (and in some cases, solute transport) at four of the commercial low-level radioactive waste disposal sites with varying degrees of success. Two of these investigations are described in other presentations of this meeting.

USGS MODELING CAPABILITIES

Models and modelers developed in the Geological Survey are capable of modeling groundwater flow in stimulated, three-dimensional, heterogeneous, anisotropic, transient conditions, on a fairly routine basis. Non-reactive solute transport, including dispersion, can be modeled under similar conditions. Transport of reactive contaminants can be modeled in two dimensions for simple linear sorption and first-order rate reactions. Multi-component reactive solutes can generally be modeled only in one dimension. Multi-component chemical equilibrium models, such as WATEQ, are used routinely for complex solutions in a non-transport mode. Flow in the unsaturated zone can be simulated for fairly simple transient non-uniform conditions with no hysteresis; however, solute transport modeling in the unsaturated zone is in its infancy. Other papers in these proceedings review the state-of-the-art in the USGS as well as other models in saturated and unsaturated groundwater conditions and in streams.

We do not yet have satisfactory modeling capabilities in the following areas:

- fractured rock systems, such as Maxey Flats, Kentucky, except for very high and/or very uniform fractures systems;
- flow in very dry, heterogeneous unsaturated zones, such as Beatty, Nevada;
- unsaturated flow with hysteresis or reactive solute transport;
- flow in any media involving complex multicomponent reactions or non-first order rate reactions;

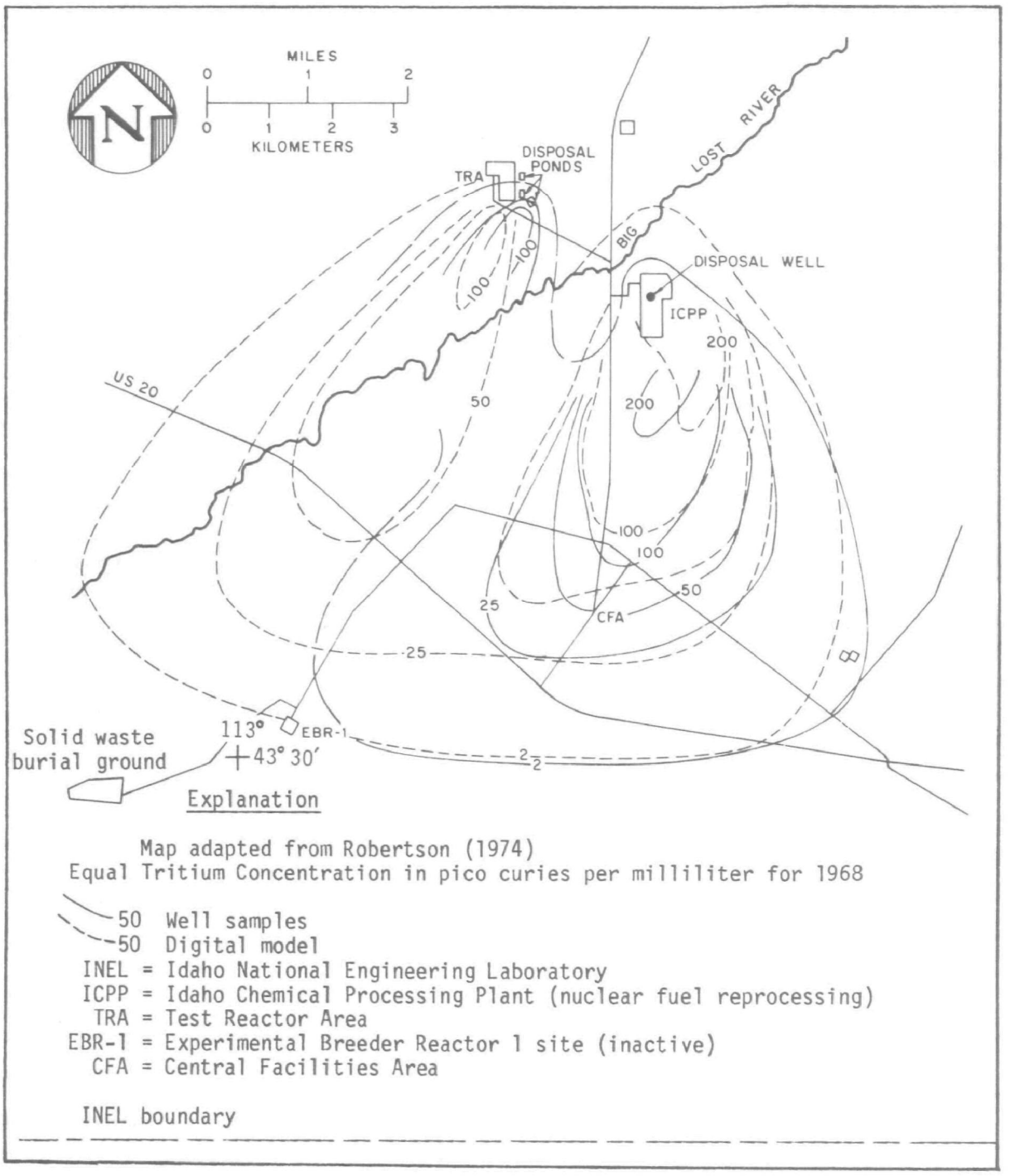

Figure 1. Comparison of ICPP-TRA waste tritium plumes in the Snake River Plain aquifer for 1968 based on well sample data and computer model.

- flow involving transport and biologically-controlled reactions.

Although these limitations are severe, we have research proceeding on all these subjects.

For most situations amenable to modeling, our models are better than our field data. Field data on dispersivity, chemical reaction parameters, and other inputs are grossly inadequate at most sites of concern. Therefore, in order to build new and better models or even to apply existing models, development of field and laboratory testing technology must proceed at comparable or faster rates. Deficiencies in our ability to measure and estimate model input parameters are actually more serious than model limitations and currently are deserving of more research attention. Related to this is a continuing need to enhance the credibility of models with many more applications and demonstrations on well-documented field problems.

CONCLUSIONS

The USGS is a strong proponent of the use of appropriate models in all hydrologic problems. The more complex the problems such as those involving waste disposal and groundwater contamination, the greater the need for modeling and the more complex are the models needed. Models are only tools to be used in conjunction with, not a substitute for, investigative analytical tools.

In waste disposal studies, the USGS needs and uses models for the following main purposes:

- to learn how to build <u>better</u> models;
- to test and confirm theories and concepts;
- to aid in managing water resources and stresses upon those resources;
- for intellectual stimulation;
- to gain competence and experience in order to advise other groups on model application;
- sensitivity analysis to screen or rank interacting processes and parameters;
- to "back-out" values of parameters such as dispersivity, distribution coefficients, and hydraulic conductivity (inverse problems);
- to gain better general insight into complex multi-component systems.

Although significant deficiencies exist in current models, the greater deficiency is in our ability to provide adequate input information to models and to demonstrate model accuracy and reliability on real field problems.

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LOW-LEVEL RADIOACTIVE WASTE MODELING NEEDS FROM THE USNRC PERSPECTIVE

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ABSTRACT

The NRC is developing a low-level waste regulation to be issued for public comment by April 30, 1981. Publication of the final rule and final EIS is expected in 1982. This regulation, 10 CFR Part 61 will apply only to near surface disposal. Two basic approaches have been considered in developing specific regulations: a prescriptive approach and a performance objective approach.

To accomplish the licensing and regulation of low-level waste disposal facilities, the information that will be needed and the methodologies to be used to assess performance are being established. Regulatory guides will cover site selection and characterization, facility design and operations, waste classification, waste form performance, site closure, post-operational surveillance, funding and monitoring. In developing licensing review procedures, initial efforts are to establish analytical modeling capabilities. We are establishing our modeling needs, determining models availability, obtaining potentially useful models and adopting those that meet our needs. As a test case, the Barnwell facility will be modeled and its performance assessed. Our analyses will then be compared with those of our contractor, ORNL and the Licensee.

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The NRC schedule for promulgation of a low-level waste regulation calls for issuance of the notice of proposed rulemaking along with a supporting draft EIS by April 30, 1981. Publication of a final rule and final EIS is expected in 1982 and will depend on the nature and extent of comments received and whether a formal hearing is held.

Part 61 will apply to the near surface disposal of waste by such means as shallow-burial, engineered structures, and deeper burial. The disposal of waste by other methods (e.g., deep mined cavity or other deep burial) will not be dealt with in this rulemaking action and will be considered at a later time through a separate rulemaking.

In developing specific regulations, we have considered two basic approaches: a prescriptive approach and a performance objective approach. In the former approach, specific detailed requirements for design and operation of a waste disposal facility would be set out in the regulations. Prescriptive standards would specify the particular practices, designs, or methods which are to be employed--for example, the thickness of the cover material (the cap) over a shallow land burial disposal trench, or the maximum slope of the trench walls.

Setting of prescriptive standards requires a considerable amount of detailed knowledge about potential designs, techniques, and procedures for disposing of waste in order to prescribe which designs, techniques, and procedures are best and also assumes that the state-of-art in waste disposal is developed to the point where there are clear choices to be made among all the potential approaches.

A regulation oriented toward performance objectives, on the other hand, would establish the overall objectives to be achieved in waste disposal and would leave flexibility in how the objectives would be achieved. The performance standards would specify levels of impact which should not be exceeded at a disposal facility in order to provide protection against radiological hazards.

NRC staff believes that neither a purely prescriptive nor a performance objective approach will be satisfactory in Part 61. A combination of both approaches is needed such that performance objectives are established to define the overall performance expected in disposal while at the same time, certain specific minimum technical criteria would be established.

NRC's overall goal is to assure protection of the public health and safety. In considering radioactive waste disposal, this goal would appear to fall into two time frames. That is, we must be concerned with protection of workers and the public during the short-term operational phase and protection of the public over the long

term after operations cease. Thus, the near-term performance objective will be to assure that the disposal facility will be operated in compliance with existing standards as set out in Part 20 of our regulations. Although routine operational releases are not expected at a disposal facility, they might occur in those cases where waste processing or volume reduction operations are conducted at a disposal site. In such cases we would propose to apply the same limits that would apply if these operations were conducted at fuel cycle facilities (40 CFR Part 190).

Assuring safety over the long term involves two considerations: 1) protection of an individual who might unknowingly contact the waste at some point in the future; and 2) protection of the general public from potential releases to the environment. We believe that intentional intrusion into the waste--e.g., an archaeologist reclaiming artifacts-cannot reasonably be protected against. After active institutional controls cease, however, one or a few individuals could inadvertently disturb the waste through such activities as construction or farming. It is important to note that consideration of intrusion involves hypothetical exposure pathways which are assumed to occur. Actual intrusion into the waste may never occur. But, for purposes of Part 61, intrusion is considered such that if it should occur the one or few individuals contacting the waste should not receive an unacceptable exposure. With respect to the unknowing intruder, we are presently considering use of the Part 20 maximum individual dose limit of 500 mrem/yr to assure protection of such an intruder.

With respect to migration and protection of the ground water, we are evaluating a range of exposure guidelines from 1 to 25 mrem/yr that would be applied at the site boundary. We expect our analyses will result in a limit around 4-5 mrem/yr.

I'd like to review what these performance objectives mean in terms establishing minimum technical requirements; that is, the prescriptive part of the regulation. These requirements would involve placing controls on the various parts or barriers of the overall disposal "system" and will determine which wastes are acceptable for near-surface disposal and which wastes are not and must therefore be disposed of by other methods providing much greater confinement. The principal parts or barriers of an overall LLW disposal system that are readily identifiable and will be addressed

in the prescriptive requirements are:

-- the characteristics of the waste and its packaging;

-- the characteristics of the site into which the waste is placed;

-- the methods by which the site is utilized, the waste emplaced and the site closed; and

-- the degree and length of institutional control, surveillance, and monitoring of the site after closure.

It is instructive to start with the intruder performance objective since although it deals with a hypothetical pathway, it provides a basis for several limiting requirements and establishes two "classes" of waste suitable for near-surface disposal.

There are two principal means of controlling potential exposures to an intruder--use of institutional controls and use of natural or engineered barriers which would make it more difficult for a potential intruder to contact the waste. Institutional controls can be further separated into two types: (1) "active" controls, which require performance of some action by a person or agency-e.g., controlled access to the site, including barries to entry (fences) and periodic inspection and monitoring of the disposal site by a regulatory or other governmental agency; and (2) "passive" controls, which are not specifically dependent upon human actions-e.g., government ownership of land, redundant records and restrictions on land use. Natural or engineered barriers could include deeper burial or use of caissons backfilled with concrete.

Neither institutional controls nor engineered barriers can be relied upon to completely prevent human intrusion. Although we have not completed our final analyses we expect to allow reliance on active institutional controls to prevent intrusion for about 100 years. This will mean that certain wastes (e.g., those with short half-lives) will not present an undue risk to an intruder when active institutional controls are removed. The active controls will be followed by several hundred additional years of passive controls.

Passive controls, although certainly minimizing potential for inadvertent intrusion may not be completely effective in preventing it. A second class of waste would then be that which may present an undue risk to an intruder when active controls are removed. For this waste additional measures must be taken to reduce this risk. This can be done by introducing an additional barrier to intrusion, such as deeper burial or engineered barriers. These additional measures will not be relied on for more than 500 years; thus waste which could potentially result in an exposure to an intruder greater than 500 mrem after 500 years is not acceptable for near surface disposal.

A similar type of analysis for migration cannot be performed in as direct a manner. While intruder exposures are relatively non-site specific, potential ground-water releases are very site specific and are more difficult to treat in as generic a fashion as the intruder. In order to carry out a site specific analysis, the variables beyond the control of the site operator need to be fixed to some extent. Of principal importance is the long-term stability of the waste and disposal facility. Unless the waste and the disposal site are stable over time, there is no way to predict the long-term radiological impacts of disposal, or the activities (maintenance, monitoring, etc.) and associated costs required to maintain potential impacts to low levels. This would suggest that all waste should be placed in a solid, non-compressible form for disposal in the near surface. However, many wastes--particularly trash waste streams--contain very low levels of activity and present little or no concern from the standpoint of long-term migration. Thus, a more reasonable requirement would be that compressible waste containing low-levels of activity should be segregated and disposed of separately. All other waste would be placed in a solid, non-compressible form (e.g., solidification in the case of resins and filter sludges) and the disposal facility should be designed and operated to enhance stability over the long-term. Certain nuclides, concentrations of nuclides or waste forms may also require individual consideration from the standpoint of migration on a site specific basis. This might include, for example, a large one-time shipment of a very mobile radionuclide or a large quantity of chelating agent in a single shipment. Thus, migration considerations establish "classes" of wastes that require special disposal considerations.

We expect to establish a common sense base of siting requirements that could be consistently applied throughout the country. The requirements would essentially eliminate certain limited areas from consideration due to undesirable characteristics leaving large areas in each region where acceptable sites could be found. The kinds of requirements we would expect to establish include:

1) Avoid areas of fractured bedrock;

2) Avoid siting in wetlands, high hazard coastal areas, floodplains, swamps or other types of very wet or potentially very wet terrain;

3) The land surface should be relatively stable structurally and geomorphically;

4) The hydrogeologic conditions of the site should be simple enough for reliable residence time prediction to be made; and

5) The site should provide long travel times for radionuclides from disposal trenches to the biosphere.

The completion of Part 61 does not, however, mean that our job is done. To accomplish the licensing and regulation of low-level waste disposal facilities, we are also establishing the information needed and the methodologies we will use to assess the performance of low-level waste disposal facilities. These efforts are concentrated in two activities--the development of regulatory guides to support the regulation and the development of licensing review procedures. The regulatory guides are being initiated more or less in parallel with our efforts on licensing review procedures. As we now envision it, regulatory guides will be developed in the areas of site selection, site characterization, facility design and operations, waste classification, waste form performance, site closure, post-operational surveillance, funding and monitoring. As with the regulation, these guides will be directed at disposal by means of shallow and intermediate depth land burial. Future guides, as needed, will be directed at other methods of disposal.

To develop our licensing review procedures, that is, the way we will review applications for low-level waste disposal, we are initially concentrating on methodologies we will use to assess performance. The first step in this development is to establish our capability to perform analytical modeling. Although NRC has extensive experience in modeling and some modeling has been done of low-level waste disposal in the past, a systematic approach is now being taken to establish a program to assure that our analytical capabilities are in place as soon as possible. To accomplish this, we have embarked on an effort to establish our modeling needs, determine the availability of models to meet these needs, obtain prospective models, develop our operational capability of the selected models, and test the models on existing or proposed sites. Let me make it clear that it is not our intention to develop a new set of models. Rather, we will investigate models that are already in use and adapt, or adopt them for our use. If our investigations reveal that there are no acceptable models to meet a specific need, we will then initiate a program of model development.

Our first task will be to develop screening criteria to be used to select potential models that can be used to simulate low-level waste sites and the effects of construction, operation and ultimate closure. Models will need to be able to simulate the geological environment, ground and surface water pathways, air pathways, biotic and vegetation pathways, radionuclide transport and the assessment of potential radiological and non-radiological impacts. Models will also be screened in terms of their level of detail and our need for such detail. In some cases site screening and gross evaluation type of models may be all that are required; whereas for other cases very detailed, highly accurate models may be needed to fully assess impacts. Perhaps in a few cases a model may need to be developed that is applicable to a specific site. The screening criteria must also take into account the need for models in a wide variety of geologic and climatic settings, e.g., the obvious differences between arid and humid sites. This screening will also be done in the context of the time and computer systems available to us.

Through our own efforts and those of our contractors and consultants, our search for available and acceptable models will begin with a review of those that NRC already has. We will also investigate what other agencies are doing and what they have available. Very specifically, this is one of the primary reasons we are here at this workshop. We are very anxious to find out what you are doing. Our efforts will also include the work going on at the National Laboratories, the universities by private industry and any other source that we can find.

As we accumulate models for potential use, we will evaluate and categorize them for our particular needs in terms of their usefulness to us for making licensing decisions. Key items in our evaluations will be:

-- their applicability (humid vs. arid sites, saturated and unsaturated flow, single and multiple aquifers, solute transport, dose assessment, etc.);

-- the details of the model (data requirements; simple, conservative vs. detailed, more realistic; difficulty of use, model options, computer requirements, etc.);

-- availability of documentation (users and programmers manuals, sample runs, examples, etc.); and

-- validation and verification of models (theoretical proofs, previous applications to field conditions, reproducibility, repeatability, etc.).

It is obvious that this is a major undertaking both in terms of time and staff effort. However, it is necessary if we are to be able to make knowledgeable licensing decisions in a timely manner. To enable us to focus on a specific goal, we have elected to concentrate our initial efforts on performing an assessment of the Barnwell Low-Level Waste Disposal Facility in South Carolina as a test case. There are several reasons why we made this choice. First, we have agreed to assist the state of South Carolina this next year in the environmental assessment of the Barnwell site as a part of their review for the renewal of the state license for the faciltiy. Second, we have contracted with Oak Ridge National Laboratory to assist us in this effort, including performance assessment of the facility. Theirs and the licensees analyses should provide a good comparison to our efforts. Last, since the Barnwell facility has been operating for some time

and there are other nuclear facilities nearby that have been studied extensively, we feel that data requirements for the selected models should probably not be a limiting factor. This should provide us more flexbility in model selection.

Once we have completed one test case (Barnwell) we will then turn over efforts to expanding our capabilities to other types of sites and situations. Hopefully, we will not have to go back to the beginning of the exercise since we should have learned a great deal the first time through and should have accumulated some applicable information.

In conclusion, I would like to summarize the modeling needs from our perspective:

1) We have identified the need for models that are directed at enabling us to make licensing decisions.

2) We have determined that the ability to perform assessments must be contained within our own staff.

3) Our modeling capabilities must be able, eventually, to evaluate the full range of potential sites, facilities, designs and operations that may occur. We have, however, elected to first concentrate on models that are potentially applicable to the Barnwell facility, which will be used as a test case.

4) We have determined that the best course for us is to adopt, or adapt, existing models to our use to the fullest extent possible.

Technical Papers

MODELING CONTAMINANT TRANSPORT IN POROUS MEDIA IN RELATION TO NUCLEAR-WASTE DISPOSAL: A REVIEW

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ABSTRACT

The modeling of solute transport in saturated porous media is reviewed as it is applied to the movement of radioactive waste in the subsurface. Those processes, both physical and chemical, that affect radionuclide movement are discussed and the references that best illustrate these processes listed. Movement is separated into convection, convection-dispersion, and convection-dispersion and chemical reactions. Solutions of equations describing such movement are divided into one-, two-, and three-dimensional analytical and numerical examples. Discussions of recent work in the area of stochastic modeling are followed by discussions of applications of the models to selected field sites.

INTRODUCTION

An important consideration in the evaluation of existing or proposed nuclear waste-disposal proposals is the impact on the environment and the exposure to man of waste material that may escape containment and be transported out of the engineered repository. For the purpose of this paper, presently available solute-transport models will be reviewed with respect to the transport of radionuclides by ground-water flow under saturated conditions from such a repository.

Mathematical modeling of radionuclide transport in porous media is the only way to quantify transport rates and discharges. The steps in modeling involve: (1) Formulation of mathematical expressions that represent the primary physical and chemical mechanisms involved; (2) determination of the parameters that appear in these expressions using measured laboratory and field data; (3) finding an acceptable method of solving these mathematical expressions; (4) evaluation of the acceptability of the formulated mathematical model in reproducing observed physical and chemical phenomena; and (5) the application of the model to the prediction of the rates of radionuclide transport and to evaluate various waste-disposal proposals. Examples and references have been selected that the authors feel best illustrate the various factors that affect such transport. The interested reader is referred to a comprehensive review by Anderson (1979) for more detailed information.

THE GENERAL EQUATIONS

Because the primary mechanism of solute transport in ground water depends on the direction and magnitude of the ground-water flow, the equation describing such flow must be formulated and solved with the appropriate boundary and initial conditions.

One form of the flow equation for a compressible fluid in a saturated nonhomogeneous anisotropic porous medium is that given by Konikow and Grove (1977) as:

$$\frac{\partial}{\partial x_i}\left[\frac{\rho k_{ij}}{\mu}\left(\frac{\partial P}{\partial x_j}+\rho g\frac{\partial z^*}{\partial x_j}\right)\right]=\rho\alpha\frac{\partial P}{\partial t}+\rho_o n\beta\frac{\partial P}{\partial t}+\frac{\varepsilon}{v_o}\sum_{k=1}^{s}\frac{\partial m_i}{\partial t}+W^*\rho^* \qquad (1)$$

where

k_{ij} is the intrinsic permeability (a second-order tensor), L^2;

ρ is the fluid density, ML^{-3};

μ is the dynamic viscosity, $ML^{-1}T^{-1}$;

P is the fluid pressure, $ML^{-1}T^{-2}$;

g is the gravitational acceleration constant, LT^{-2};

z^* is the elevation of the reference point above a standard datum, L;

$W^* = W^*(x,y,z,t)$ is the volume flux per unit volume (positive sign for outflow and negative for inflow), T^{-1};

ρ^* is the density of the source/sink fluid, ML^{-3};

α is the vertical compressibility coefficient of the medium, $LM^{-1}T^2$;

ρ_o is the fluid density at a reference pressure, temperature, and concentration, ML^{-3};

n is the total porosity for compressive storage (dimensionless);

ε is the effective porosity (dimensionless);

β is the compressibility coefficient of the fluid, $LM^{-1}T^2$;

v_o is the reference volume of the fluid, L^3;

m_k is the mass of species k in the reference volume v_o, M;

s is the number of species, (dimensionless);

x_i are the cartesian coordinates, L; and

t is time, T.

The equation for transport of a dissolved chemical species can be obtained by combining the principle of the conservation of mass with Fick's law of diffusion. Assumptions that result in the following equation can be found in Konikow and Grove (1977):

$$\varepsilon \frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(\varepsilon D_{ij} \frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(\varepsilon C V_i\right) - C'W^* + \sum_{k=1}^{S} R_k \qquad (2)$$

where

- C is the concentration of the solute species in the flowing phase, ML^{-3};
- ε is the effective porosity of the medium;
- D_{ij} is the hydrodynamic dispersion coefficient (a tensor), L^2T^{-1};
- V_i is the interstitial velocity, LT^{-1};
- W^* is the volumetric flow rate/unit volume of porous medium of a source/sink, T^{-1};
- C' is the concentration of the species in the source/sink flow, ML^{-3}; and
- R_k is the rate of production of solute species in the kth reaction $T^{-1}L^{-3}$.

Once the set of reactions described by R_k is specified, equation (2) can be written for each chemical species of a system and the set of equations solved simultaneously with the flow equation. The boundary conditions for the solute-transport equation include boundaries along which the solute concentration is specified, and those along which continuity of the flux of the solute species is required. Initial conditions specifying the solute-concentration distributions must be given for all species.

The primary coupling of the flow equation to the solute-transport equation is through the interstitial velocity obtained from Darcy's law. The back-coupling or effect of the transport equation on the flow equation is through the dependence of fluid density and viscosity on solute concentration.

For instances where the solute concentrations are very dilute it commonly is assumed that the fluid density and viscosity are constant. The flow equation can then be solved independently from the transport equation. In essence, the presence of the chemical-solute species does not affect the flow field, but the flow field is still the primary mechanism for solute transport.

For studies where a two-dimensional areal model is appropriate, the above equation can be integrated in the vertical direction throughout the saturated thickness of the aquifer. Such situations occur when horizontal ground-water movement is much larger than vertical movement.

TRANSPORT MECHANISMS

The primary solute-transport mechanism is the flow of ground water resulting in convection of the solute species, and is represented by the second term on the right hand side of equation (2).

Hydrodynamic dispersion, a secondary transport mechanism, describes the net macroscopic transport effect of movements of the individual solute particles through the porous medium, Bear (1972). Hydrodynamic dispersion consists of two processes. One is diffusion of solute on the molecular scale described by a Fickian diffusion term with a molecular-diffusion coefficient. The other is mechanical dispersion that describes transport due to the variations of velocity across individual pores, and the mixing of fluid at pore junctions. The two coefficients usually are lumped together and the mechanical dispersion dominates in all but the slowest of flow systems.

Scheidegger (1961) relates the dispersion coefficient to the interstitial velocity by the equation:

$$D_{ij} = a_{ijmn} \frac{V_m V_n}{|V|} \tag{3}$$

where

a_{ijmn} is the dispersivity or characteristic length of the porous medium (a fourth-order tensor), L;

V_m and V_n are the components of the flow velocity of the fluid in the m and n direction, respectively, LT^{-1}; and

$|V|$ is the magnitude of the velocity vector, LT^{-1}.

When the coordinate system is aligned with the average velocity in a steady, uniform flow field in an isotropic medium, the dispersion coefficient tensor reduces to two components, a longitudinal and a transverse coefficient (Scheidegger, 1961, and Bachmat and Bear, 1964, and Bredehoeft, 1969).

Recent analyses (Smith and Schwartz, 1980) of the dispersive effects caused by macroscale heterogeneities in the permeability of a porous medium, have shown that dispersion of solute at this scale is not described by a Fickian diffusion term.

Transport and the associated dispersion and diffusion through fractures, where there may be a flowing and a stagnant fluid phase, can be analyzed using the concept of dead-end pores and is discussed by De Smedt and Wierenga (1979).

CHEMICAL REACTIONS

The reaction term includes all chemical processes that can occur during transport (Back and Cherry, 1976). These may include homogeneous reactions that occur within the fluid phase and heterogeneous reactions that take place between the solid and liquid phases.

An example of a common homogeneous reaction is an irreversible rate reaction such as radioactive decay. In this instance the reaction rate term R in equation 2 becomes:

$$R = - \lambda(\varepsilon c + \rho_b \bar{c}) \tag{4}$$

where

λ is the radioactive-decay constant (equals ln 2/half life), T^{-1}; and

$\bar{c}$ is the concentration of the species adsorbed on the solid (mass of solute/mass of sediment), ML^{-3}.

Heterogeneous reactions include sorption ion exchange, diffusion into a stagnant fluid phase with possible sorption or reaction, precipitation and dissolution. When heterogeneous reactions are being considered, a separate mass balance equation for the sorbed or stagnant phase must be solved simultaneously with equation (2). For the simple heterogeneous reaction such as equilibrium-controlled sorption or ion exchange with a linear adsorption isotherm the reaction rate term for a single species can be written as:

$$R = - K_d \rho_b \frac{\partial c}{\partial t} \tag{5}$$

where

K_d is the distribution coefficient that defines the relationship between the dissolved and adsorbed ions.

Grove (1976) and Enfield and others (1976) discuss basic forms of sorption and ion-exchange mechanisms. The sorption mechanisms that have been simulated to date include kinetically controlled sorption and equilibrium sorption.

MATHEMATICAL MODELS OF SOLUTE TRANSPORT

The solutions to the governing equations of flow and solute transport for a given system geometry, boundary conditions, initial conditions, and reaction-mechanism procedure form the mathematical model of the system. The following sections summarize transport models that have been developed which are relevant to nuclear-waste disposal. Analytical and numerical solutions to the models are discussed separately with these being further subdivided under the headings of (1) convection, (2) convection-dispersion, and (3) convection-dispersion and chemical reactions. When appropriate, the types of models are further divided according to dimensionality.

Analytical Models

Convection. The transport model for convection only in one dimension is trivial as the output matches the input with only a time delay for travel. For two dimensions, in a horizontal plane, Nelson (1978a, 1978b) gives several examples for travel times and concentration changes during solute movement from a source to an outflow boundary.

Convection-dispersion. For the convection-dispersion model in one dimension the flow field is usually taken as uniform and steady, thus eliminating the need to solve the flow equation. Bear (1972) presents some solutions for a variety of boundary conditions and source terms for this case. Other solutions include those of Brenner (1962), Lindstrom and Boersma (1971), Gelhar and Collins (1971), and Al-Niami and Rushton (1977). For two dimensions, solutions are presented by Bear (1972), Sauty (1980) and Fried and Combarnous (1971). For the cases of radial transport and equation transformation of equations to simpler forms, results are available from Bear and Jacobs (1965), Bear (1972), Hoopes and Harleman (1967), and Phillips and Gelhar (1978).

Convection-dispersion-reaction. Examples of one-dimensional solutions that involve linear homogeneous reactions are given by Bear (1972), Marino (1974a), and Parlange and Starr (1978). Two-dimensional examples with similar reactions have been presented by Hunt (1973, 1974). Many one-dimensional transport models have been developed for various heterogeneous reactions. Examples for linear equilibrium sorption and linear kinetically-controlled sorption are given by Lapidus and Amundson (1952), Ogata (1964), Girshon and Nir (1969), Marino (1974a, 1974b) and Enfield and others (1976). An analytical transport model for a three-member radionuclide decay chain with linear equilibrium sorption and an impulse or decaying-slug source terms has been derived by Lester and others (1975). The cases of both dispersive and nondispersive transport were treated. Nondispersive transport was examined in a similar manner by Rosinger and Tremaine (1978). Details of the numerical implementation of the model are given by Kipp (1979) and DeMier and others (1979).

Examples of analytical solutions for two-dimensional transport including kinetic sorption and decay are presented by Eldor and Dagan (1972) and Wilson and Miller (1978).

Numerical Models

Convection. The one-dimensional convective-transport case with constant interstitial velocity can be solved analytically and is of no interest numerically. For two dimensions Nelson (1978c, 1978d) gives several good examples of modeling convective-transport and transient-flow systems.

Convection-dispersion. The numerical solution of the solute-transport equation with dispersion can be quite difficult because of numerical-diffusion errors and solution oscillations caused by the

particular technique. Because of these problems a variety of numerical techniques have been used. These include finite-difference and finite-element methods and the method of characteristics (MOC). Examples illustrating these problems and the use of various methods to minimize numerical dispersion (Lantz, 1971) and oscillations have been proposed by Stone and Brian (1963), Chaudari (1971), and Chhatwal and others (1973). Examples of finite-element methods used to overcome such difficulties for one-dimensional problems are given by Price and others (1968), Pinder and Shapiro (1979) and Van Genuchten and Gray (1978). Huyakorn (1977) proposed using an upwind finite-element method to overcome the oscillation problem in convection-dominated transport. Pinder and Cooper (1970) and Reddell and Sunada (1970) describe the method of characteristics/particle in cell model for transport calculations that overcomes numerical-dispersion and overshoot/undershoot problems. A description of the U.S. Geological Survey's MOC model is given by Konikow and Bredehoeft (1978).

Peaceman and Rachford (1955, 1962) presented one of the first finite-difference numerical techniques for two-dimensional transport. Several of the finite-difference formulations cited previously have been extended to two-dimensional problems with convective and dispersive transport.

Many two-dimensional finite-element based solute-transport models have been developed. Guymon (1970) used a variational principle; Nalluswami and others (1972) included the mixed partial-derivative terms; Pinder (1973) used the Galerkin technique; and Smith and others (1973) demonstrated the greater generality of the Galerkin technique over variational formulations. Lee and Cheng (1974) and Segol and others (1975) used a finite-element method to solve the density dependent coupled flow and solute-transport equations.

Huyakorn and Taylor (1977) compared the relative merits of the velocity-pressure formulation, the stream-function formulation, and the hydraulic-potential formulation for the coupled flow and solute-transport problem and found the first method to be the most accurate, yet the most expensive.

The three-dimensional solute-transport models with dispersion and convection include Khaleel and Reddell's (1977) and Reddell and Sunada's (1970) method of characteristics model and Gupta and others (1975) finite-element model.

Convection-dispersion-reaction. The numerical simulation of convection, dispersion, and reaction of chemical species through porous media in most instances simply involves the addition of the reaction term on the convection-dispersion equation. While most applications of this are for one-dimensional column experiments the extension of the principle to two- and three-dimensional systems is quite straight forward.

The one-dimensional PERCOL model of Routson and Serne (1972) treats convective transport with equilibrium reactions of a set of "macroions" (ions present in high concentrations). It then computes the transport of microions (ions present in low concentrations), which are radionuclides present in small concentrations and undergo equilibrium sorption. The sorption coefficients are a function of the macroion concentrations.

The MMT1D radionuclide-transport model of Washburn and others (1980) computes the transport of N-member radionuclide decay chains and includes linear equilibrium-sorption with constant sorption coefficients. The dispersive transport is simulated by a discrete parcel random-walk technique described by Ahlstrom and others (1977). Hill and Grimwood (1978) also developed a one-dimensional model of radionuclide-chain transport with linear equilibrium sorption and radioactive decay.

Finite-difference techniques are illustrated by Lai and Jurinak (1972) and finite-element methods by Rubin and James (1973). Both solve the general differential equation with linear or nonlinear reactions.

An early two-dimensional transport model with chemical reactions was that of Schwartz and Domenico (1973); it used finite differences, neglected dispersion, but treated a multiplicity of chemical reactions including both equilibrium and kinetic. The REFQS model of Shaffer and Ribbens (1974) also calculated the transport of several chemical species using the same techniques as Schwartz and Domenico, but included dispersive transport.

Schwartz (1975) developed a radionuclide transport method-of-characteristics model which included binary cation exchange and linear decay. Finite-element techniques were used by Duguid and Reeves (1976) to simulate transport with equilibrium sorption and linear decay; by Prakash (1976) for transport in a bounded radial-flow system for a partially penetrating well; by Cabrera and Marino (1976) for two-dimensional flow and transport in a stream-aquifer system; by Pickens and others (1979) for transport to tile drains; and by Pickins and Lennox (1976) for a steady free surface-flow system with constant equilibrium sorption.

Ahlstrom and others (1977) presented the Discrete Parcel Random Walk transport model, MMT-DPRW, which is an extension of the particle-in-cell method in that the dispersive transport is simulated by a statistical random-walk computation. The idea of a numerical random-walk simulation for dispersive transport in porous media also was used by Todorovic (1975). A cell grid is used and parcels of fluid are tracked during the simulations. The model can incorporate the chemical reaction computations performed by Routson and Serne's (1972) PERCOL.

The case of flow in a fractured medium with diffusion into adjacent porous blocks, including linear equilibrium sorption and linear decay mechanisms, has been investigated using finite elements by Grisak and Pickens (1980).

Three-dimensional flow systems with solute transport are difficult to model numerically because of the large number of computational nodes involved, even for systems of moderate size. An approximate method of treating this problem was given by Ross and Koplik (1979) who perform the one-dimensional transport calculations with equilibrium sorption and linear decay along steady-state streamtubes generated by an appropriate three-dimensional flow model. A convolution integration with the analytical Green's function solution is used to obtain the concentration field.

The INTERA (Intercomp Resource Development and Engineering, Inc., 1976, INTERA Environmental Consultants, Inc., 1979) three-dimensional flow, solute- and energy-transport model is a fully coupled flow and transport simulation code using finite-difference techniques. Linear equilibrium sorption and linear decay for single-species transport is included. This model was extended to handle radionuclide-decay chains and named SWIFT (Dillon and others, 1978). The radionuclide species are assumed to be in dilute solution and thus do not affect the flow field.

COMPUTATIONAL PROBLEMS IN SOLUTE TRANSPORT MODELING

With analytical-solution models, the only difficulties that may arise are roundoff errors, overflows in certain function evaluations, and insufficient accuracy in numerical quadrature. The first two problems can be resolved by combining terms in the proper order. This is particularly necessary in the radionuclide-chain calculations. Accurate numerical quadrature can usually be achieved by using an adaptive method and isolating any significant peaks of the integrand.

With finite-difference and finite-element models there is the possibility of excessive numerical dispersion (Oster and others, 1970; Lantz, 1971) oscillation in the solution due to the space- or time-discretization method, (Price and others, 1966), and overshoot/undershoot near a steep concentration gradient (Gray and Pinder, 1976). Oscillation and overshoot/undershoot are probably related if not the same thing. As mentioned above, various correction terms have been used to minimize numerical dispersion. The method of characteristics was developed to avoid this problem.

Oscillation problems can be avoided by proper selection of time- and space-step sizes (Price and others, 1966; Siemieniuch and Gladwell, 1978) but restrictions may make a given computation quite impractical. Higher order time-integration methods have been proposed to avoid oscillation problems, for example, Norsett methods (Smith and others, 1977). Overshoot/undershoot occurs because a finite-difference or finite-element representation cannot propagate all frequencies contained in the solution-function representation at the same phase speed or without attenuation (Gray and Pinder, 1976). One of the advantages of finite-element methods is that the use of higher-order basis functions gives better propagation behavior over a wider range of frequencies. Higher-order basis functions minimize numerical instabilities but cost more in computer-solution time (Grove, 1977).

Discrete-parcel tracking or Lagrangian-simulation techniques are oscillation free and nearly free from numerical dispersion and are mass conservative at the cost of a slower computation and the presence of some random noise errors from the dispersion calculation (Ahlstrom and others, 1977).

The main problems with three-dimensional models are the computation-time and computer-storage requirements. This is particularly true if transport of multiple species are being simulated. Fast and efficient equation solvers for the matrix equations generated have been developed and are being improved. Out-of-core matrix storage is another technique being used to minimize core-storage requirements. At the present time however, many of the larger three-dimensional problems can only be run on large, very fast computers.

STOCHASTIC CONCEPTS IN SOLUTE TRANSPORT MODELING

It has long been realized that there is uncertainty in the description of the physical and chemical properties of the porous medium. To collect sufficient data on a real system for a precise deterministic model is an impossible task. Thus, some effort has been made to attempt to quantify the uncertainty in transport-model prediction and correlate it with the uncertainty in the various model parameters. Only a few results have been achieved to date. A group of studies involved the modeling of large-scale dispersion by using macroscopically variable hydraulic-conductivity fields (Warren and Skiba, 1964; Heller, 1972; Schwartz, 1977; Smith and Schwartz, 1980). The models used tracer-particle tracking techniques with a one-dimensional mean flow field. Results of these studies showed that a unique dispersivity cannot be defined when the low-permeability inclusions are not arranged homogeneously. Smith and Schwartz (1980) found that even with statistically homogeneous conductivity fields, the tracer particles do not take on a normal distribution and a constant dispersivity does not exist. Also, a large uncertainty is associated with the predicted solute elution curve even when the statistical features of the porous medium are known.

Gelhar and others (1979) looked at longitudinal dispersion due to variations in hydraulic conductivity in a stratified porous medium. They developed a stochastic differential equation describing the system and used spectral techniques to solve it. The transient nature of the dispersion process and non-Fickian dispersion effects were identified.

All of the above studies show that, unless sufficient transport time has elapsed, dispersion due to large scale heterogeneities of the porous medium does not obey the deterministic Fickian type mechanism.

FIELD APPLICATION OF TRANSPORT MODELS

Low-level radioactive waste-disposal sites are being thoroughly studied by the U.S. Geological Survey as well as other Federal and State agencies. Although a qualitative knowledge as to what is going on at

these sites is usually known, a quantitative understanding of contaminant movement, both within and off site, generally is lacking. Such movement can be studied through the use of the ground-water solute-transport models discussed earlier. As mentioned, a wide variety of models are available for use. However, examples of field applications using such models available in the general literature are somewhat limited.

There are, however, several situations where modeling has been applied to the movement of chemical species in ground water with good results. Although those discussed in the following paragraphs are not exhaustive they are representative of "state-of-the-art" applications. Discussions of each field site will be brief and interested readers are referred to the references for more detail.

As was mentioned previously, solution of the solute-transport equation presents significant mathematical problems that must be overcome by fairly sophisticated solution methods. For this reason the first studies of field applications used a particle-tracking technique that was entitled the method of characteristics (MOC). The technique was used by Bredehoeft and Pinder (1973) who studied the salt-water contamination of a limestone aquifer at Brunswick, Georgia. The source of the contamination was underlying brackish water migrating upward through natural conduits in response to lowered hydraulic heads in the overlying aquifers. Simulation studies showed interceptor wells to be the most feasible method to protect the well field. This reference also provides an extensive theoretical background to the partial differential equations that describe solute transport.

Konikow and Bredehoeft (1974) investigated salinity increases in ground water and surface water in an alluvial valley in southeastern Colorado as related to irrigation practices. The MOC model was used. Dissolved-solids concentrations calculated by the model were within 10 percent of the measured values for both the aquifer and stream approximately 80 percent of the time.

Konikow (1976) used this same model to reproduce the 30-year history of chloride contamination at the Rocky Mountain Arsenal, Colorado. Here, liquid industrial waste had seeped out of unlined disposal ponds and spread over many square miles in an alluvial aquifer.

Robson (1974) used the MOC to model the water quality of a shallow alluvial aquifer near Barstow, California. The aquifer had been polluted by percolation of wastes and sewage from industrial and municipal sources for about 60 years. Several strategies to alleviate the pollution problem and to protect downgradient domestic wells were investigated by model simulation. Robson (1978) also modeled the same system in a vertical section. This model has the advantage of being able to simulate vertical flow and water quality changes in a single- or multiple-aquifer system.

Robertson (1974) used a MOC water-quality model to predict the migration of industrial and radioactive liquid wastes throughout a 15-square-mile area at the Idaho National Engineering Laboratories (INEL) in Idaho. The wastes were disposed of in the Snake River Plain aquifer. Chloride and tritium were found to have moved as far as 5 miles downgradient from the injection point. Strontium-90 and cesium-137 were significantly retarded due to sorption. The strontium was detected no more than 1.5 miles downgradient and cesium migration was not detected. All of the above species were adequately simulated using the MOC model and estimates made of the long-term effects of these contaminants on aquifer usage. Robertson (1977) also modeled solute transport from waste seepage ponds at INEL. A three-segment numerical model, incorporating analytical and multidimensional numerical solutions, was used in this study.

Grove (1977) used a two-dimensional finite-element solute-transport code to simulate the same data from Robertson's (1974) study. Virtually the same results were obtained using this numerical technique.

Pinder used the finite-element method to simulate several field situations of water-quality change. A chromate contamination problem at Long Island, New York was well simulated by Pinder (1973). He also simulated the two-dimensional movement of a saltwater front in the Cutler area of the Biscayne aquifer near Miami, Florida (Pinder, 1975). Due to the density effect caused by the saltwater concentrations, a set of non-linear partial differential equations had to be solved simultaneously.

Cheng (1975) used a finite-element method to study the movement of variable-density fluids through a causeway dividing the Great Salt Lake in Utah. The model did not match concentration variables measured in the field, but it did give some insight into the hydrology of the system.

Ahlstrom and others (1977) documented the theoretical foundation and numerical-solution procedure for the Hanford MMT-DPRW model. A simulation of the tritium plume beneath the Hanford, Washington site was included to illustrate the use of the model in a typical application.

CONCLUSION

It is clear from the review of available ground-water solute-transport models for saturated flow systems that many of the basic mechanisms that apply to real site situations can be simulated with certain simplifying assumptions. Analytical models are adequate for parameter-sensitivity analyses and preliminary investigations of transport phenomena, particularly when there is a gross lack of field data for model-parameter determination. The simplifying assumptions necessary for analytical solutions restrict their ability to realistically model a real system. Numerical models have the ability to treat the more complicated systems such as heterogeneous porous media. However, determining the parameter distributions for a real system from a sparse data set can be fraught with uncertainties that limit the quality of the model predictions.

Areas where the modeling technology need further development include flow and transport in fractured/porous media, transport of multiple chemical species with complex chemical and sorptive interactions, and transport modeling using stochastic principles in order to handle the uncertainties in real systems.

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AN OPTIMUM MODEL TO PREDICT RADIONUCLIDE TRANSPORT IN AN AQUIFER FOR THE APPLICATION TO HEALTH EFFECTS EVALUATIONS

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ABSTRACT

This paper presents an optimum groundwater transport model for simulating radionuclide transport in an aquifer using an approximate solution of the basic transport equation. The model is designed to avoid (1) relatively high computer simulation costs normally experienced in numerical models and (2) the large errors which are sometimes introduced when the physical boundary conditions are converted to a mathematical form suitable for an analytical model. The model neglects the effect of radionuclide transport through dispersion first and then compensates for this effect later with a health effects correction factor. This correction factor is found to be a function of the Peclete number and the "transport number," which has been defined, and can be determined by using the parameters of the groundwater transport system. The model has a low cost of simulation and yet maintaining reasonable accuracy for the peak and cumulative radionuclide discharges, which are of primary interest for risk assessments. Preliminary analyses indicated that the model can be integrated into most of the risk assessment models for health effects evaluations.

INTRODUCTION

Comprehensive studies on the evaluation of the optimum method of disposal of radioactive wastes have been conducted by various government agencies [1,2] and by an Interagency Review Group [3]. All of these studies have unanimously concluded that the geological disposal method is one of the most viable alternatives. Because transport through an aquifer is a primary pathway of transporting radionuclides to the biosphere, a groundwater model which simulates the migration of radionuclides in an aquifer is one of the important transport submodels employed for health effects evaluation.

To date, there are more than one hundred and eight groundwater transport models [4]. However, some of the models fail to consider the process of radioactive decay and/or sorption and are, therefore, not

suitable for application to health effects evaluations. The rest of the models which may be suitable for health effects evaluation can be subdivided into two groups: the analytical model and the numerical model. In general, analytical models are limited by specific mathematical boundary conditions which require some approximation of actual physical conditions [5, 6, 7]. As a result, these models suffer considerable error in simulation due to these approximations.

The application of a numerical model requires, in general, many more tedious computations than the analytical approach does. Besides, the accuracy of simulation depends greatly on the adjustments of time and space increments; severe errors may result if they are improperly adjusted. On the other hand, a proper adjustment of these increments, in some cases, may result in excessive computer time required for the simulation. The cost may become prohibitive when the model is applied to long-term simulations such as health effects evaluations.

The purpose of this study is to present a groundwater transport model which could overcome the shortcomings of existing models and to characterize the model when it is applied in health effects evaluations.

APPLICATION OF EXISTING MODEL IN HEALTH EFFECTS EVALUATIONS

The basic equations for a groundwater transport system include the momentum, the energy and the continuity equations for the hydrodynamic system, and the continuity equation for the solute and the constituent radionuclide in a decay chain. Using tensor notations, the equations take the form:[12]

$$\underline{v} = -(k/\mu)(\nabla p - \rho g \nabla z) \tag{1}$$

$$\nabla\cdot[(\rho k/\mu)H(\nabla p - \rho g\nabla z)] + \nabla\cdot\underline{\underline{D}}_h\cdot\nabla T - q_L - q'H = (\partial/\partial t)[\eta\rho U + (1-\eta)(\rho C_p T)] \tag{2}$$

$$\nabla\rho\underline{v} + q' = -(\partial/\partial t)(\eta\rho) \tag{3}$$

$$\nabla\cdot[\rho C(k/\mu)(\nabla p - \rho g\nabla z)] + \eta\nabla\cdot\rho\underline{\underline{D}}_c\cdot\nabla C - q'C - \rho\eta\lambda_d RC = (\partial/\partial t)(\rho\eta RC) \tag{4}$$

in which C is the concentration of the radionuclide in the fluid phase; $\underline{v}$ is the velocity vector; k is the permeability; μ is the viscosity of the fluid; p is the pressure; ρ is the mass density; g is the gravitational acceleration; D is the dispersivity tensor; T is the temperature; q_L is the rate of heat loss; H is the fluid enthalpy; η is the porosity; z is the height above reference plane; λ_d is the decay constant; R is the retardation factor; U is the internal energy; C_p is the specific heat; q' is the rate of fluid withdrawal; and subscripts h and c are the heat energy and component of mass respectively.

The above non-linear equations characterize the transport of radionuclides in the groundwater system. Since each of the above equations are related through dependent variables, the direct solution of the system equation for any boundary and initial conditions is extremely difficult and not practical. A commonly used practice in solving the system equation is to assume that the flow of groundwater is steady and that there is no heat energy being generated or absorbed in the system. The system equation then reduces to a single equation.

$$R(\partial C/\partial t) - \nabla\cdot(\underline{\underline{D}}\cdot\nabla C) + V\nabla C + \lambda_d RC = 0 \qquad (5)$$

in which V is the interstitial velocity ($V = v/n$). Equation (5) has been further simplified and solved by numerous authors [7, 8, 9] employing numerical or analytical approaches. The difficulties encountered in applying these models for health effects assessments are described in the following sections.

Numerical Models

The existing multidimensional models are solved either by the finite difference method [8] or by the finite-element method [9]. Although a model employing the finite-element method is, in general, found to be more efficient than one employing the finite difference method [10], the time required to execute a computer model employing the finite element method is still far beyond the limitations of a normal project budget for risk assessment when a number of cases must be considered.

The simulation of the vertical migration of tritium from a burial trench toward the groundwater table conducted for the West Valley, New York burial site [11] used finite element model developed by Duguid and Reeves [9]. Approximately seven minutes of computer process time was required on UNIVAC-110 computer for simulating 200 years of real time. The analysis also indicated that the half strength concentration ($C/Co = 0.5$) wave front moved 0.6 m in 20 years. Assuming that 1000 years of real time is required to simulate the system and that the time required for the simulation of the radionuclide migration in a groundwater stream is the same as that for the vertical migration, then the total time required for simulating the West Valley or similar groundwater system would be 700 min for completing simulation of ten critical radionuclides. This is equivalent to $10,500 per run, a cost that is unquestionably excessive.

A one-dimensional INTERA model [12] developed by INTERA Environmental Consultants, Inc., employs a finite difference method. It has a computer processing cost of $200 for simulating the migration of a single radionuclide in a one mile long aquifer for a 100,000 years real time simulation. This is also too costly when many other radionuclides and pathways are to be considered for a complete health effects evaluation.

Analytical Models

Lester, Jansen, and Buckholder developed an analytical groundwater transport model for a one-dimensional, semi-infinite aquifer system which has impulse release and decay step release boundary conditions [6]. These boundary conditions at x = 0 are expressed mathematically as

$$C = C_0\delta(t) \tag{6}$$

and

$$C = (C_0/t_d)\exp(-\lambda_d t) \tag{7}$$

for the impulse release and the decaying step release, respectively. In the above equation, x is the space coordinate, t is the time, t_d is the duration of radionuclide leaching, and C_0 is the concentration of radionuclides at t = 0.

Ford, Bacon, and Davis, Inc., developed an analytical model which assumed that the rate of radionuclide release at any time is proportional to the inventory of radionuclides remaining at the source point. Mathematically, it is expressed as

$$C = (\lambda_L I_m/Q_w)\exp[-\lambda_d + \lambda_L)t] \tag{8}$$

in which λ_L is the leaching constant, I_m is the initial inventory of the radionuclides in the waste depository, and Q_w is the rate of groundwater flow.

These analytical models have made considerable contributions in groundwater transport modeling by simplifying the procedures of simulation. However, the application of these models to health effects assessments is limited because it requires the approximation of converting the physical boundary condition to a form meeting the requirements of an analytical model. This may result in considerable error of simulation in some cases.

The above discussion implies that existing numerical and analytical groundwater models may either be too costly to compute or may introduce large errors when applied to health effects assessments. Therefore, a more accurate and more economic groundwater transport model has been developed for health risk assessment and is presented herein.

THEORETICAL BACKGROUND OF THE OPTIMUM GROUNDWATER TRANSPORT MODEL FOR HEALTH EFFECTS EVALUATIONS

Derivation of Basic Equation

This transport model is intended to simulate a uniform, one-dimensional flow in an aquifer. It receives radionuclides released from

the waste disposal site and transports them to the biosphere for biological uptake. This includes wells, springs, streams, and other use and discharge points. It is assumed that the dissolved raionuclides are in sorption equilibrium with the aquifer formation and that decay is in progress for both dissolved and sorbed radionuclides.

The basic one-dimensional groundwater transport equation for the model simulating radionuclide migration in an aquifer may be reduced from Eq. (4) to

$$D(\partial^2 C/\partial x^2) - V(\partial C/\partial x) - R(\partial C/\partial t) - \lambda_d Rc = 0 \tag{9}$$

and should be solved by using the following initial and boundary conditions:

$$C = 0, \quad \text{at all } x, \quad \text{when } t = 0, \tag{10}$$

$$C = C_0(t), \quad \text{at all } x, \quad \text{when } t > 0, \tag{11}$$

$$C = \text{finite}, \quad \text{at } x = \infty \quad \text{when } t > 0$$

For the convenience of health effects analysis, one may convert the radionuclide concentration, C, into the rate of radionuclide transport by multiplying Eqs. (9), (10), and (11) by the rate of groundwater flow. When this transformation is completed, Eqs. (10) and (11) become:

$$D(\partial^2 \dot{Q}/\partial x^2) - V(\partial \dot{Q}/\partial x) - R(\partial \dot{Q}/\partial t) - R\lambda_d \dot{Q} = 0 \tag{12}$$

$$\dot{Q} = 0, \quad \text{at all } x, \quad \text{when } t = 0,$$

$$\dot{Q} = Q_0(t), \quad \text{at } x = 0, \quad \text{when } t > 0, \text{ and} \tag{13}$$

$$\dot{Q} \text{ finite, CyH} \quad \text{at } x = \infty, \quad \text{when } t > 0$$

where $\dot{Q}$ denotes the rate of radionuclide transport.

Since Eq. (13) is an undefined boundary condition, the analytical solution for Eq. (12) cannot be obtained. However, its solution can be expressed in an integral form by employing the method of Green's function, that is:

$$\dot{Q}(t) = \int_0^t \dot{Q}_0(t - \tau)u(\tau)d\tau \tag{14}$$

in which u denotes the radionuclide release rate at the discharge end, x = L, which responds to the unit release of a radionuclide at x = 0 and τ is a dummy variable of time.

The response of unit release in Eq. (14), $u(\tau)$, has been thoroughly studied by Burkholder et al. [6] with the following results:

$$u(\tau) = (V/2L)\sqrt{(RP/\pi\Theta^3)}\,\text{Exp}\{-N_d\Theta - (P\Theta/4R)[(R/\Theta) - 1]^2\} \tag{15}$$

in which P is the Peclet number (= VL/D); Θ is the dimensionless time (= $\tau V/L$); Nd is the decay number (= $\lambda_d L/V$). By substituting Eq. (15) into Eq. (14) one obtains.

$$\dot{Q}(t) = \int_0^t \dot{Q}_0(t-\tau)\ (V/2L)\sqrt{(RP/\pi\theta^3)}\ \mathrm{Exp}\{-N_d\theta-(P\theta/4R)[(R/\theta)-1]^2\}d\tau \tag{16}$$

Equation (16) can not be integrated because $Q_0(t-\tau)$ is undefined. However, if the dispersion term, $D(\partial^2\dot{Q}/\partial x^2)$, in Eq. (12) is neglected, then this response of unit release, $u(\tau)$ can be simplified and becomes [6]

$$u'(\tau) = \mathrm{Exp}(-RL\lambda_d/V)\delta(\tau - RL/V) \tag{17}$$

As a consequence, Eq. (14) can be integrated and the result is

$$\dot{Q}'(t) = \mathrm{Exp}(-RL\lambda_d/V)\dot{Q}_0(t - RL/V) \tag{18}$$

In Eqs. (17) and (18), δ denotes the delta function, and the prime on u' and $\dot{Q}'$ denotes variables in which the dispersion term has been neglected.

Although Eq. (18) is easier to calculate than Eq. (16), the results computed from Eq. (18) include an error resulting from neglecting the dispersion term in the basic transport equation. In order to compensate for this error, a correction factor defined by

$$\xi(P,R\lambda_d L/V,t) = \dot{Q}(t)/\dot{Q}'(t) \tag{19}$$

has been introduced. When this correction factor is characterized, the rate of radionuclide transport $\dot{Q}(t)$ may also be computed from:

$$\dot{Q}(t) = \xi\mathrm{Exp}(-RL\lambda_d/V)\dot{Q}_0(t - RL/V) \tag{20}$$

which is obtained from the combination of Eq. (19) and Eq. (18).

In Eq. (20), the correction factor ξ is expected to be a function of t, P, and $R\lambda_d L/v$; the complexity of this term prohibits its use. Nevertheless, since the end goal of health effects assessments is aimed at estimating fatal health effects, which are primarily determined by the cumulative health effects resulting from the lifetime dose rather than by the annual dose rate, one may also introduce a long-term health effects correction factor, η, defined as:

$$\eta = \mathrm{THE}/\mathrm{THE} \tag{21}$$

where THE and THE represent the total health effects obtained from the groundwater pathway at the discharge end with and without considering the dispersion term, respectively.

In addition, let us assume that the total health effects due to the released radionuclides are so small that they would not alter the size of the population at risk and other factors affecting the health effects.

If this is the case, there is a linear relationship between the cumulative radionuclides released and the expected total health effects which is governed by the health effects conversion factors [13]. Thus, Eq. (21) can be rewritten as:

$$\eta = [HECF_0 \int^{\infty} \dot{Q}(t)dt]/[HECF_0 \int^{\infty} \dot{Q}'(t)dt] \tag{22}$$

where HECF represents the health effects conversion factor. Subsequent substitution of Eq. (14) into Eq. (22) yields

$$\eta = [_0\int^{\infty} {}_0\int^{t} \dot{Q}_0(t-\tau)u(\tau)d\tau dt]/[_0\int^{\infty} {}_0\int^{t} \dot{Q}_0(t-\tau)u'(\tau)d\tau dt] \tag{23}$$

Since no radionuclides are being released at x = 0, when t<0, the upper limit of the integration in Eq. (23) may be converted from time t to infinity without changing the results of the integration. Thus, Eq. (23) may be rewritten as:

$$\eta = [_0\int^{\infty} {}_0\int^{\infty} \dot{Q}_0(t-\tau)u(\tau)d\tau dt]/[_0\int^{\infty} {}_0\int^{\infty} \dot{Q}_0(t-\tau)u'(\tau)d\tau dt] \tag{24}$$

Now, since the time integral of the functions $Q_0(t-\tau)$ and $u(\tau)$ converge to finite numbers when t is infinite, Eq. (24) can be transformed to

$$\begin{aligned}\eta &= [_0\int^{\infty} u(\tau)d\tau \, {}_0\int^{\infty} \dot{Q}_0(t-\tau)dt]/[_0\int^{\infty} u'(\tau)d\tau \, {}_0\int^{\infty} \dot{Q}_0(t-\tau)dt] \\ &= [_0\int^{\infty} u(\tau)d\tau]/[_0\int^{\infty} u'(\tau)d\tau]\end{aligned} \tag{25}$$

Equation (25) implies that the health effects correction factor η is independent of environmental time and, hence, can be characterized independent of time. Once the health effects correction factor is determined, the rate of radionuclide release at the discharge end may be approximated by:

$$\dot{Q}(t) = \eta Exp(-RL\lambda_d/V)\dot{Q}_0(t - RL/V) \tag{26}$$

Equation (26) is the basic equation of this groundwater transport model.

Characterization of Health Effects Correction Factor

To determine the characteristics of the health effects correction factor, one may substitute Eqs. (15) and (17) into Eq. (25) and then complete the integration of the denominator. This yields

$$\eta = \frac{_0\int^{\infty} (1/2)\sqrt{(RP/\rho\theta^3)}Exp[-N_d\theta - (P\theta/4R)(R/\theta - 1)^2]d\theta}{Exp(-RL\lambda_d/V)} \tag{27}$$

A series of computations were made for the numerator and the denominator of Eq. (27), using various values for P, Nd, and R. The error between the results of analysis obtained for the denominator and for the numerator were also computed and extended to evaluate the relative error.

Careful examination of the results reveal that the relative error is a primary function of the Peclet number and the parameter expressed by $R\lambda_d L/V$. This parameter represents the ratio of the radioactive decay constant, λ_d, and the "transport constant," V/RL, and is designated as "transport number" for this study. The above results were plotted on a Peclet number vs. transport number plane as shown in Fig. 1. This figure indicates that the relative error, ε, increases with the increase in transport number and decreases with the increase in Peclet number.

Based on the definition of relative error, the health effects correction factor can be computed by

$$\eta = 1 + \varepsilon \tag{28}$$

Since the relative error is always greater than 0, the health effects correction factor is always greater than 1.

Proposed Groundwater Transport Model for Health Effects Assessment

Based on the previous discussions a groundwater system with initial and boundary conditions as shown in Eq. (13) may be simulated by Eq. (26), which is duplicated as;

$$\dot{Q}(t) = \eta \text{Exp}(-RL\lambda_d/V)\dot{Q}_0(t - RL/V) \tag{29}$$

Equation (29) represents an algebraic equation, in which, constant η is determined from Fig. 1 and Eq. (28); and the terms, RL/V and λ_d are also known constants determined from the characteristics of the groundwater system. Therefore, the proposed model described by Eq. (26) is the simplest and most economical to process when it is integrated into a health effects assessment model.

It should be noted that when this model is employed in a health effects assessment model, there may be some error in the health effects for each generation. The size of this error depends on the characteristics of the system, the nature of the radionuclide being considered, and the boundary conditions. The nature of this error is characterized in the following section. Nevertheless, the cumulative health effects evaluated for each generation, based on this model, is expected to be a insignificant error relative to the true solution obtained from the one dimensional model expressed in Eqs. (9), (10), and (11). This fact is also discussed in the following section.

CHARACTERIZATION OF THE POTENTIAL ERROR OF THE PROPOSED MODEL

Hypothetical Groundwater System

In order to characterize the nature of error incurred by the proposed model, a hypothetical groundwater transport system was established.

In the hypothetical groundwater system, it was assumed that: the velocity of groundwater flow is 100 m/yr; the location of radionuclide discharge is 500 m down stream from the source point where the radionuclide is released; the coefficient of dispersion is 300 m^2/yr; the rate of radionuclide release at the source point, x = 0, varies with time and is represented by

$$\begin{aligned} \dot{Q}_0(t) &= \text{Sin}[(\pi/t_d)t] && \text{for } 0 \le t \le t_d \\ \dot{Q}_0(t) &= 0 && \text{for } t > t_d \end{aligned} \tag{30}$$

where t_d is the duration of radionuclide release.

Three cases are assumed for the analysis. Case I represents a fast release, t_d = 200 yr, and long radionuclide half-life, λ_d = 0.000693. Case II represents a fast release, t_d = 200 yr, and short radionuclide half-life λ_d = 0.0693. Case III represents a slower release, t_d = 400 yr, and long radionuclide half-life, λ_d = 0.000693. Each case is also subdivided into three subcases with the retardation factors equal to 1, 10, and 100, respectively.

Method and Results of Analysis

Two models were developed for the analysis. One of them was developed based on a numerical integration of Eq. (16) and was designated the "Exact Model." The other model was developed based on Eq. (29) and was designated as the "Optimum Model." Each of these models were designated to compute the radionuclide discharge rate at the downstream end of the aquifer and the cumulative radionuclides released at the discharging point over infinite time. The results of computer analyses using these two models are presented in Figs. 2, 3, and 4.

Discussion of Results

In case of long radionuclide half-life, Cases I and III, the rate of radionuclide release and the cumulative radionuclide release computed from the exact model and the optimum model agree very well for all three subcases assumed. However, the results of the Case II analysis, where the radionuclide half-life is short, indicate, that the rate of radionuclide discharge obtained from the optimum model deviates more and more from that obtained from the exact model as the retardation factor increases. Nevertheless, the major deviations are merely in the time-lag of radionuclide discharge, whereas the peak discharge showed little deviation (Fig. 3). The results of this latter analysis also indicated that the above deviation will be mitigated for those radionuclides with longer half-life, i.e., with smaller transport number (Fig. 2). Fortunately, a system with larger transport numbers results in a limited quantity of radionuclide discharge at its discharging point as can be seen by comparing case II-3 versus cases II-2

or II-1. This result implies that the discharge of radionuclides under a high transport number, such as Case II-3, would not be a major concern from the view point of health effects assessment. Besides, this deviation should further decrease with the increase in the duration of radionuclide release at the radionuclide source point, x = 0, as shown in Figs. 2 and 4.

Nevertheless, the cumulative radioactive discharge, which is the primary parameter in determining the total health effects from a radioactive waste disposal site, remains the same for values obtained from the exact model and from the optimum model. This agreement implies that the proposed optimum groundwater transport model can be integrated into the health effects assessment model without introducing any significant error in the assessment of health effects.

CONCLUSION

An optimum groundwater transport model for health effects assessment has been derived and characterized. The processing time required to simulate this model is significantly less than for other comparable models because it only requires algebraic calculations.

The error from simulating the peak discharge of radionuclides using the "optimum" model, as compared with the error from use of the "exact" model [i.e., the numerical model represented by Eqs. (16) and (30)], may be noticeable when the groundwater transport number is greater than 5. However, the cumulative radionuclides released under the same conditions is normally only a small fraction of the cumulative radionuclides released at the source point. Therefore, the effect of this error is mitigated.

The error in assessment of health effects from the proposed optimum model, as compared to that obtained from an exact model, has been found to be is insignificant in practical applications.

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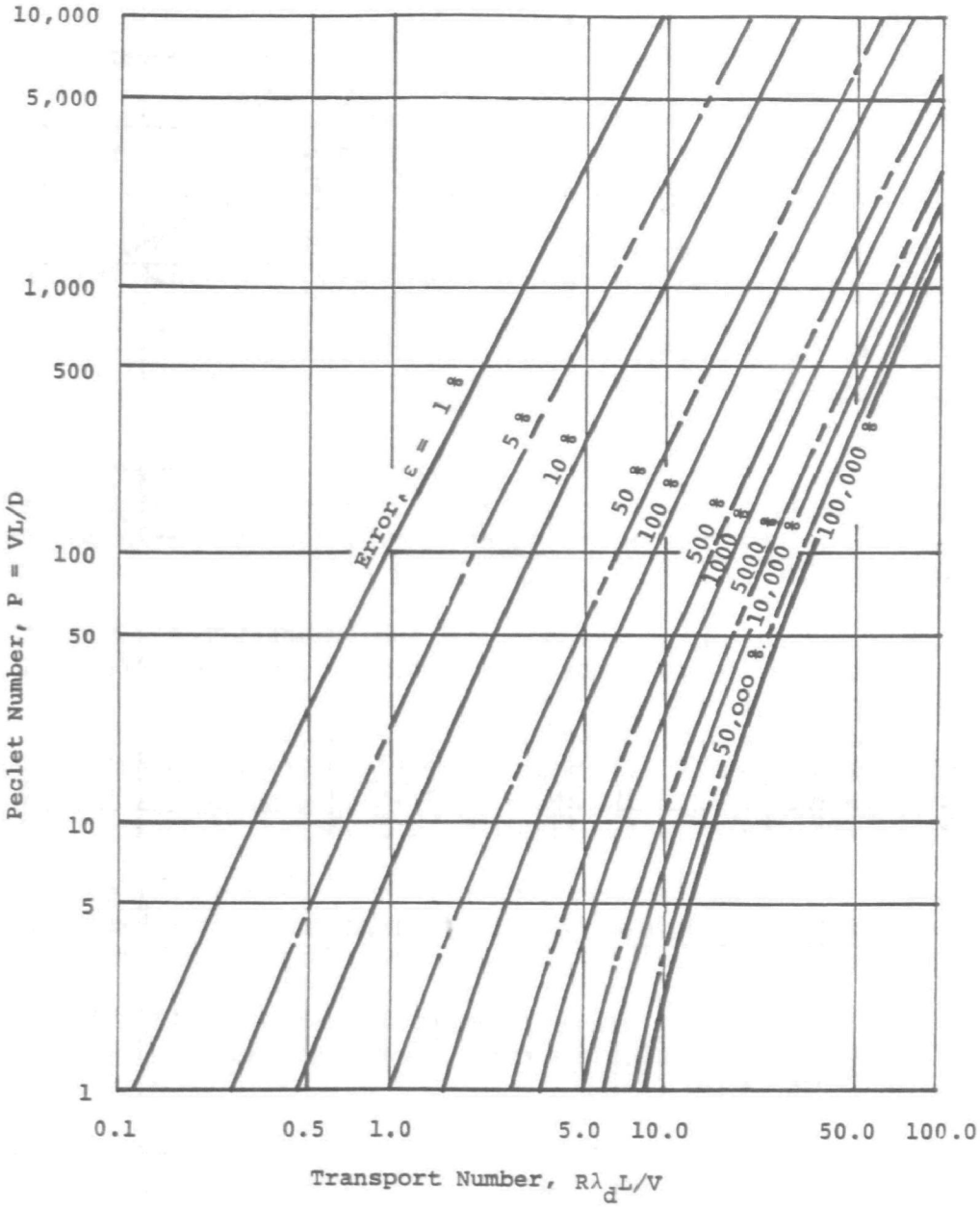

Fig. 1. Results of the Health Effects Correction Factor Analysis Using Eqs. (27) and (28).

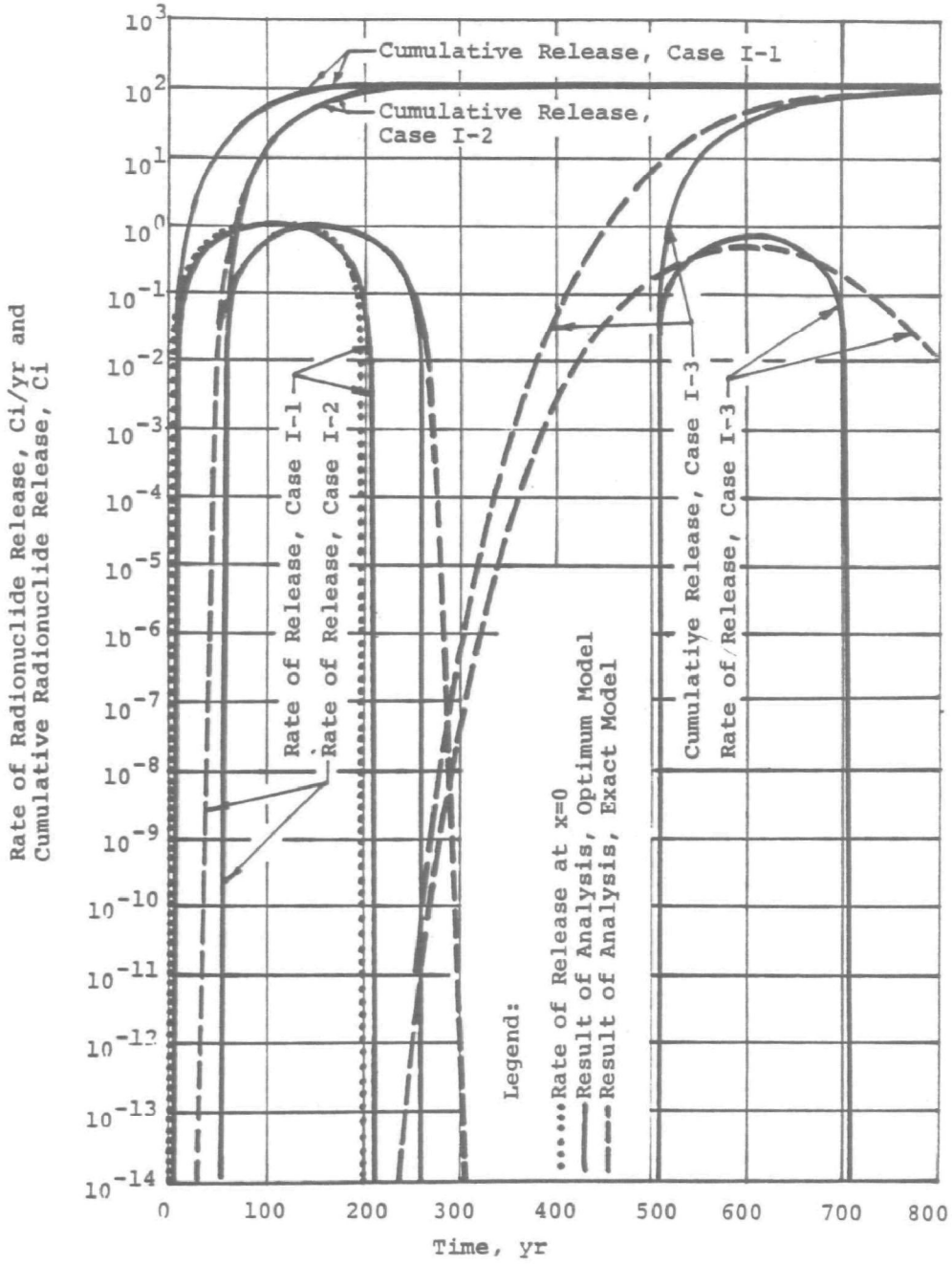

Fig. 2. Comparison of the Results of Analyses Obtained from the Optimum Model and the Exact Model, Case I, λ_d = 0.000693, t_d = 200 yrs.

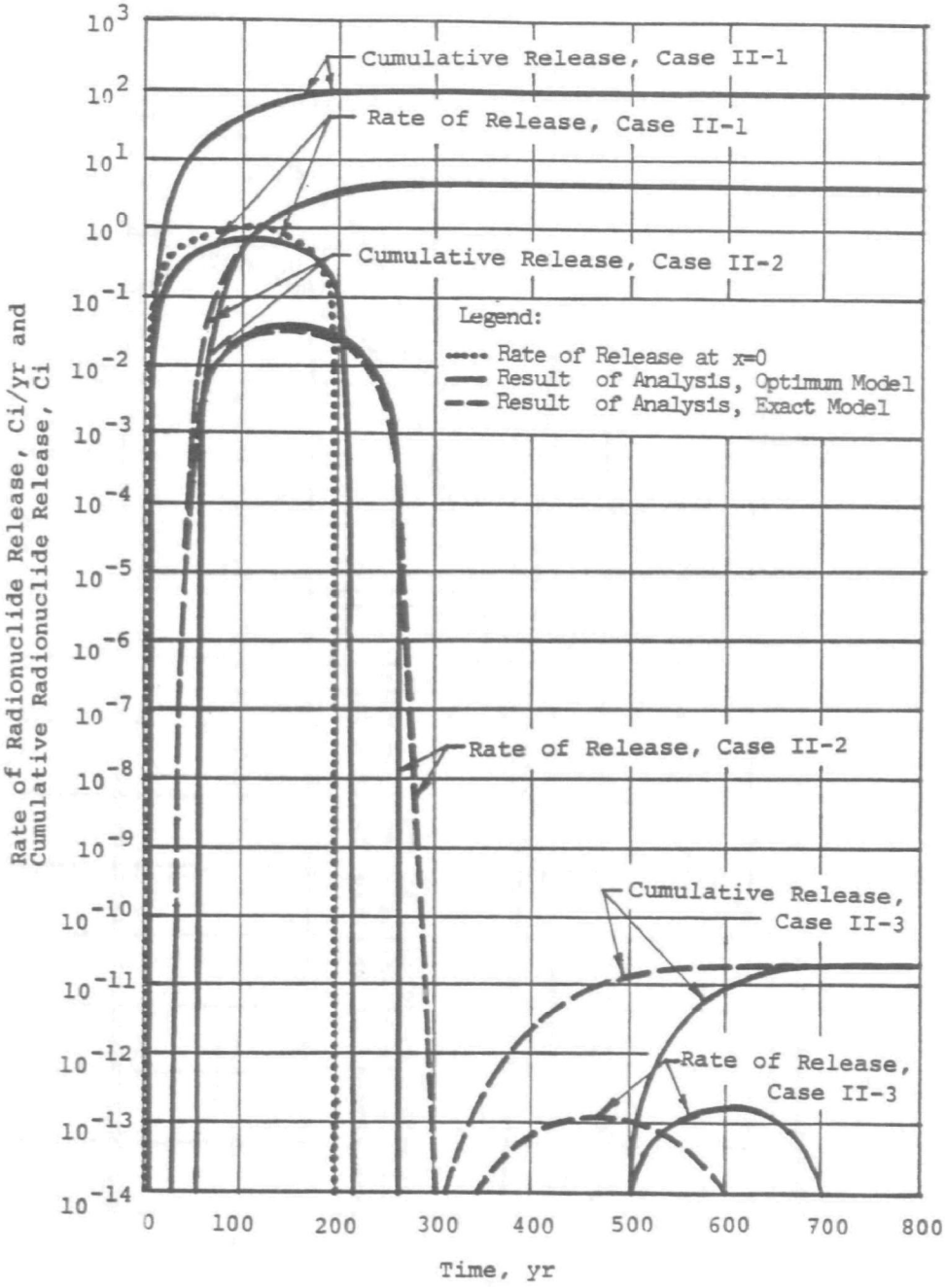

Fig. 3. Comparison of the Results of Analyses Obtained from the Optimum Model and the Exact Model Case II, $\lambda_d = 0.0693$, $t_d = 200$ yrs.

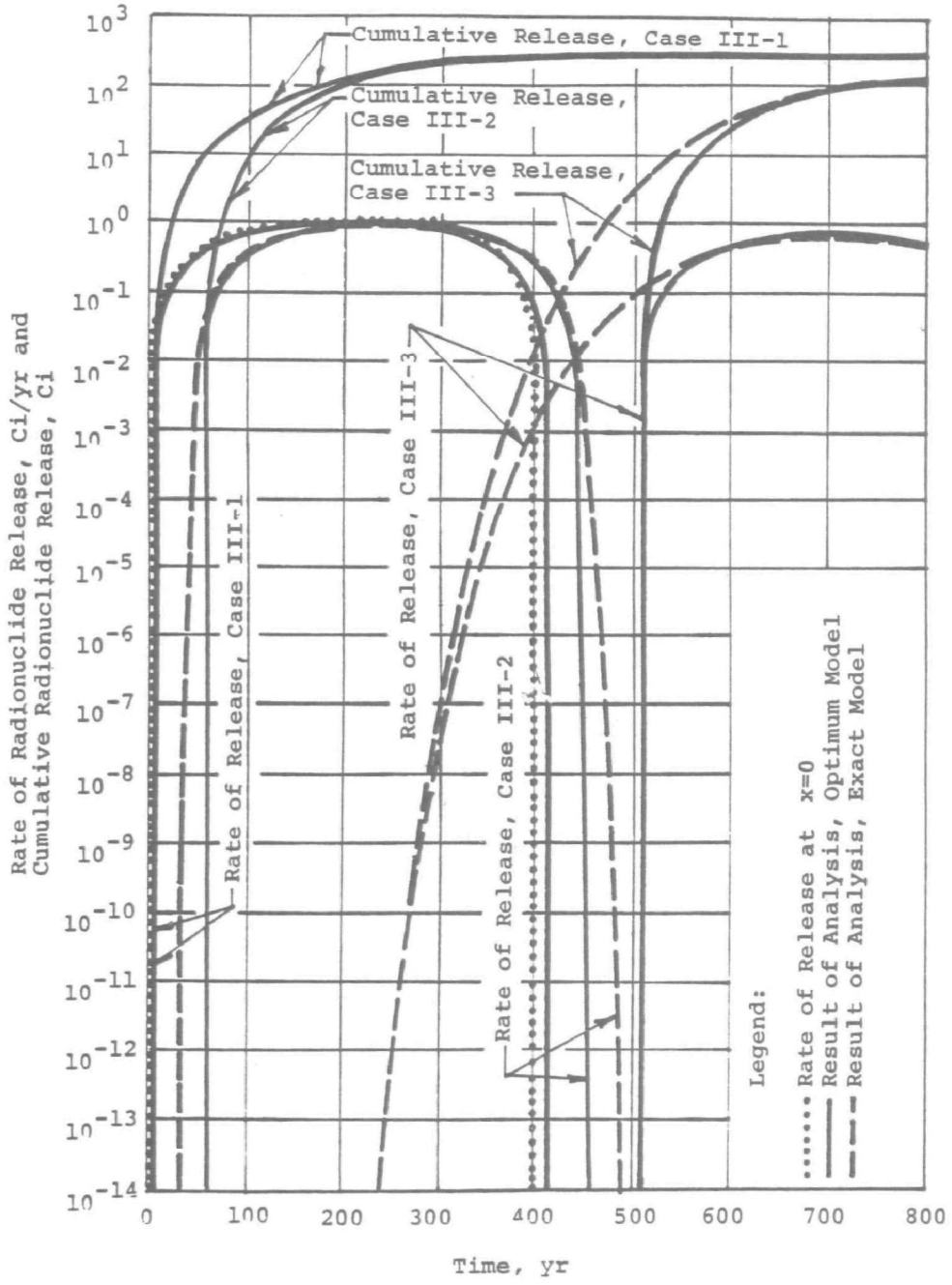

Fig. 4. Comparison of the Results of Analyses Obtained from the Optimum Model and the Exact Model, Case II, λ_d = 0.000693, t_d = 400 yrs.

MODELING OF WATER AND SOLUTE TRANSPORT UNDER VARIABLY SATURATED CONDITIONS: STATE OF THE ART

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ABSTRACT

This paper reviews the equations used in deterministic models of mass and energy transport in variably saturated porous media. Analytic, quasi-analytic, and numerical solution methods to the nonlinear forms of transport equations are discussed with respect to their advantages and limitations.

The factors that influence the selection of a modeling method are discussed in this paper; they include the following:

1. The degree of coupling required among the equations describing the transport of liquids, gases, solutes, and energy;
2. The inclusion of an advection term in the equations;
3. The existence of sharp fronts;
4. The degree of nonlinearity and hysteresis in the transport coefficients and boundary conditions;
5. The existence of complex boundaries; and
6. The availability and reliability of data required by the models.

Analytic solutions are available for a variety of steady-state nonlinear multidimensional problems such as infiltration of liquid water from point or line sources. Analytic treatment of heterogeneity and anisotropy is limited to spatial variations in material properties (such as exponential dependence of hydraulic conductivity with depth) that are not generally realistic. Some quasi-analytic methods are numerically unstable, leading to oscillatory solutions, and in a few cases, convergence to the wrong solution. The principal advantage of existing analytic and quasi-analytic methods is in deriving general conclusions about the nature of solutions that may be used to check the validity of numeric methods based on finite differences or finite elements.

Numeric methods are reviewed as they have been applied to variably saturated transport problems. The preferred method with the most flexibility for extremely nonlinear water-flow problems is a finite difference scheme applied to the balance equation, written in terms of pressure or total head, with upstream weighting on the relative hydraulic conductivity.

In addition, nonlinear coefficients should be evaulated implicitly and improved by iteration. Galerkin finite element schemes may result in oscillatory and non-convergent solutions to these problems. Finite element methods based on orthogonal collocation somewhat reduce these problems. However, the advantage of increased accuracy of finite element schemes over finite difference schemes is reduced by the large computer times required to formulate and solve the resulting algebraic equations. Finite element schemes appear to be preferred for linear and mildly nonlinear forms of the transport equations when sharp fronts are involved. Verified, documented computer codes that use both finite element and finite difference schemes are available for a variety of realistic problems that arise in designing and managing waste disposal sites. However, use of these models is not routine because of numeric problems of solving the descriptive equations. Consequently, most problems should be analyzed with more than one approach or model to assure consistency.

INTRODUCTION

Quantitative description of movement of water and solutes through variably saturated porous media is required to enable adequate design and management of waste-disposal sites. Water originating as precipitation or irrigation water percolates through overburden and the waste itself. This water may dissolve pollutants which may reach underlying aquifers or streams and lakes by downward and lateral movement. In addition, gaseous waste forms may escape to the biosphere via upward diffusion. Thus, the timing and location of pollutant loadings to potable water supplies and the biosphere require quantitative description of the movement of recharge waters, dissolved solutes, and gaseous pollutants.

Since this movement occurs through porous and fractured media that may or may not be totally saturated with water, a three-phase system comprising moist air, water, and solids must be analyzed. The equations describing water and solute movement in these systems are complicated; their solution usually requires some type of numerical approximation. These approximations, the required transport coefficients, and initial and boundary conditions comprise a model of a particular field problem. Field problems generally include heterogeneity in the transport coefficients and boundary conditions that vary in both time and space.

Until recently, solutions to these equations for realistic field problems were impossible; however, with the development of modern computers, many realistic problems can be analyzed. It is the purpose of this paper to: (1) review the equations involved in variably saturated mass and energy transport and the principal modeling methods that have been used for the solution of these equations; (2) present problems encountered in the principal solution methods; and (3) present needs for future work in the application of models incorporating these methods. About 330 reports on solutions to the equations for transport of mass and energy in variably

saturated systems were reviewed. Primary emphasis of the review was on problems involving flow of liquid water and dissolved solutes. However, some discussion of problems involving combined movement of heat and moisture in both liquid and vapor phases, and gaseous diffusion is included. Some of the references through 1971 include comprehensive reviews by other authors (Braester and others, 1971). Problems of transport in systems that are saturated at all times will be covered in another paper at this symposium (Grove and Kipp, 1980).

BASIC TRANSPORT EQUATIONS

Physics-based models of movement of water, solutes, and heat through variably saturated porous or fractured media are derived by combining mathematical statements of the conservation of mass and energy with constitutive equations relating these statements to measurable variables, such as pressure, temperature, and concentration. These equations are generally written to apply over some finite space in which the transport properties are constant or over which they can be assumed to vary in some simple manner. The continuity of mass equation is:

$$\int_V S_m \frac{d\rho}{dt} dV = \int_S q_m dS \qquad (1)$$

where

S_m = a general mass storage coefficient,

ρ = the mass density,

t = time,

V = volume of the region considered,

S = surface of the region considered,

q_m = the mass flux density orthogonal to the surface S.

A similar equation for the balance of energy is:

$$\int_V S_H \frac{dh}{dt} dV = \int_S q_h dS \qquad (2)$$

where

S_H = a general enthalpy storage coefficient,

h = energy content or enthalpy,

q_h = enthalpy flux.

Constitutive equations that relate mass and energy flux to measurable variables state that the flux is proportional to the first power of a driving force which is expressed as a gradient in the measurable variable. For the flux of liquid water (q_ℓ), a generalized Darcy's law is the appropriate equation:

$$q_\ell = - \rho_\ell \left\{ K_p \left[\nabla\phi_p + \nabla\phi_g \right] + K_h \nabla\phi_h + K_o \nabla\phi_o \right\}_\ell \qquad (3)$$

where

ρ_ℓ = mass density of liquid water,

K_p = liquid hydraulic conductivity coefficient,

K_h = conductivity for thermally induced liquid flux,

K_o = conductivity for osmotically induced liquid flux,

ϕ_p, ϕ_g, ϕ_h, and ϕ_o are pressure, gravitational, thermal, and osmotic potentials,

∇ = gradient operator,

ℓ = subscript to indicate liquid water.

In most applications, the only potentials of significance are the first three. Osmotic potential may be important where materials are present that act as semipermeable membranes.

A similar equation for the flux of moist air (q_a), neglecting all driving forces except gradients in pressure and thermal potentials, is:

$$q_a = - \rho_a \left\{ K_p \left[\nabla\phi_p + \nabla\phi_h \right] \right\}_a, \qquad (4)$$

where all terms are as described above with the subscript a for air replacing ℓ for water.

The flux of gases, including water vapor, and solutes dissolved in liquid water (q_m) in response to a concentration gradient is described by Fick's law:

$$q_m = - L \nabla\rho_c \qquad (5)$$

where

L is a general coefficient that accounts for the effects of diffusion and hydrodynamic dispersion (Bear, 1972), and

ρ_c is the mass concentration of the gas or solute.

This formulation of Fick's law using mass concentration is valid for diffusion of a constituent of a low enough concentration that the mass of the solvent is not appreciably affected by the presence of the solute. For most cases relative to waste disposal, this is true; one exception is in the treatment of coupled heat and water-vapor flow under high temperatures. In this case, when water vapor moves due to a concentration gradient, the concentration should be expressed as a mass fraction (mass of water vapor as a ratio to mass of moist air).

When a moving fluid is involved, an advection term is added to the righthand side of equation 5:

$$q_m = - L \nabla \rho_c + q_f \rho_c \tag{6}$$

where

q_f = volumetric flux rate of the solvent fluid.

The flux of enthalpy (q_h) due to heat conduction and advection of enthalpy in a moving fluid is described by adding an advection term to Fourier's law:

$$q_h = - \lambda \nabla T + C_p \rho_f T q_f \tag{7}$$

where

λ is a general thermal conductivity,

T is the temperature,

C_p is the mass specific heat, and

ρ_f is fluid density.

If phase changes are involved, the latent heat of vaporization or the heat of fusion must be accounted for by incorporating them in the general thermal conductivity, and in the advection term (in the case of latent heat).

Combining equations 3–7 with equations 1 and 2 and adding source/sink terms results in the following balance equations for liquid water, moist air, water vapor, or gaseous pollutants, solutes, and enthalpy, that are applicable to most field problems in waste disposal.

Liquid water

$$\int_v S_\ell \frac{d\rho_\ell}{dt} dV + \int_s \rho_\ell K_p \{ \nabla \phi_p + \nabla \phi_g \}_\ell + K_h \nabla \phi_h \quad dS + \int_v Q_\ell \, dV = 0 \tag{8}$$

Moist air

$$\int_v S_a \frac{d\rho_a}{dt} dV + \int_s \rho_a K_a \{\nabla\phi_p + \nabla\phi_h\}_a dS + \int_v Q_a dV = 0 \quad (9)$$

Water vapor or gaseous pollutants

$$\int_v S_g \frac{d\rho_g}{dt} dV + \int_s \{L_g \nabla\rho_g - q_a \rho_g\} dS + \int_v Q_g dV = 0 \quad (10)$$

Solutes dissolved in liquid water

$$\int_v S_s \frac{d\rho_s}{dt} dV + \int_s \{L_s \nabla\rho_s - q_\omega \rho_s\} dS + \int_v Q_s dV = 0 \quad (11)$$

Flux of energy

$$\int_v S_H \frac{dT}{dt} dV + \int_s \{\lambda \nabla T - C_p \rho_f T q_f\} dS + \int_v Q_H = 0 \quad (12)$$

The source/sink term in equations 8-12 is generally a function of space, time, and perhaps temperature, pressure, or concentration. Equations 8-12 along with appropriate boundary and initial conditions and measured or derived values of the transport coefficients comprise the basis of models applicable to field problems. Boundary conditions are required to specify the solution variable(s) or the flux of mass or energy across the boundary of the modeled region as a function of time and space. Examples are specified concentration at a contaminant source, rainfall rate, and heat flux from a canister containing spent nuclear fuel.

Equations 8-12 are partial differential equations that may be nonlinear owing to the dependence of the transport coefficients, boundary conditions, and (or) source/sink terms on the solution variable. It is principally the nonlinear nature of these equations when they are applied to variably saturated flow problems that requires extension of the solution methods and applicable models from those used for linear problems. The nonlinearity in the transport coefficients is exemplified by the general hydraulic conductivity in equation 8, which is a function of properties of fluid, medium, and pressure potential:

$$K_{p\ell} = \frac{\bar{\bar{K}}}{\mu_\ell} K_r (\psi) \quad (13)$$

where

$\bar{\bar{K}}$ = the intrinsic permeability of the medium, L^2,

μ_ℓ = dynamic viscosity of water, $ML^{-1}T^{-1}$,

K_r = a relative conductivity which depends upon the capillary pressure potential (ψ) dimensionless,

ψ = the difference between air pressure (P_a) and liquid pressure ($P_{\omega\ell}$) energy/unit mass.

Figure 1 shows typical functions of K_r for a sand and clay.

The general storage coefficient in the water flux equation is also highly nonlinear and depends upon the capillary pressure potential (fig. 2). The transport coefficients in the energy flux equation are also nonlinear because of their temperature dependence. Nonlinearity in the transport coefficients is further exacerbated when coupled equations are used. For example, in a coupled water-flux solute-transport problem, hydraulic conductivity of the medium may be affected by the solute concentration; as, for example, when waters high in sodium infiltrate soils containing clay minerals (Frankel and others, 1978; Pupiski and Shainberg, 1979). Another example is the strong temperature dependence of dynamic viscosity in the water flux equation for coupled heat and moisture flow problems.

In addition to nonlinearity in transport coefficients, certain boundary conditions may cause the equations being solved to be nonlinear. An example would be isothermal evaporation, where the evaporative flux depends upon the unknown pressure head in the soil immediately below the land surface. Source/sink terms may be nonlinear also; examples would be the rate of water uptake by a plant root system, which depends on the unknown pressure potential in the soil surrounding the root, and sorption of a contaminant species which depends upon the solute concentration. Table 1 shows the degree of nonlinearity generally associated with equations 8-10 as they might be applied to variably saturated conditions at a waste-disposal site.

MODELING APPROACHES

Depending upon the problem being analyzed, any subset of equations 8-12 may be required to describe the physical system.

The solution of the equations that are part of a model of a given field problem may be accomplished in one of three ways: (1) By use of analytic or quasi-analytic methods; (2) by use of an analog model such as resistance-capacitance networks or deformable membranes; (3) by the use of approximate numerical techniques. Because of the nonlinearities in equations 8-14, analog models have found very limited application. Since only one reference to the use of electric analog model to analyze variably saturated flow problems was found (Bouwer and Little, 1959), further discussion of analog models will be omitted.

Although analytic and numeric solution methods will be discussed separately, this subdivision is arbitrary. In general, analytic methods utilize direct integration or series solutions to equations 8-12, and treat time and space as continuous; numeric methods involve discretization of the solution domain and the time span of interest into finite intervals. A section is also included on parametric or input-output models that may incorporate some features of both analytic and numeric methods.

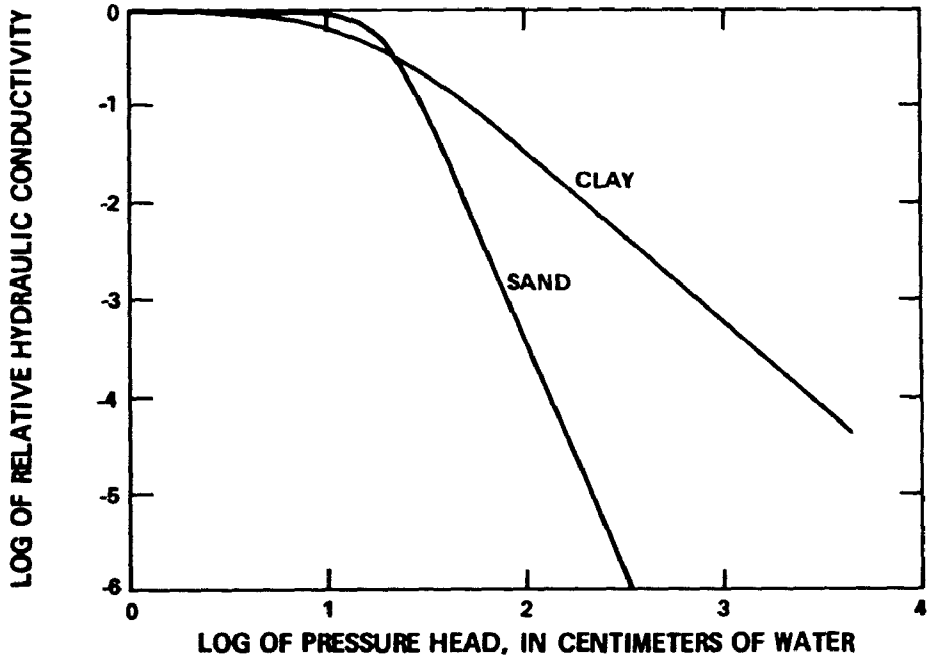

Figure 1. -- Relative hydraulic conductivity to liquid water for a sand and clay.

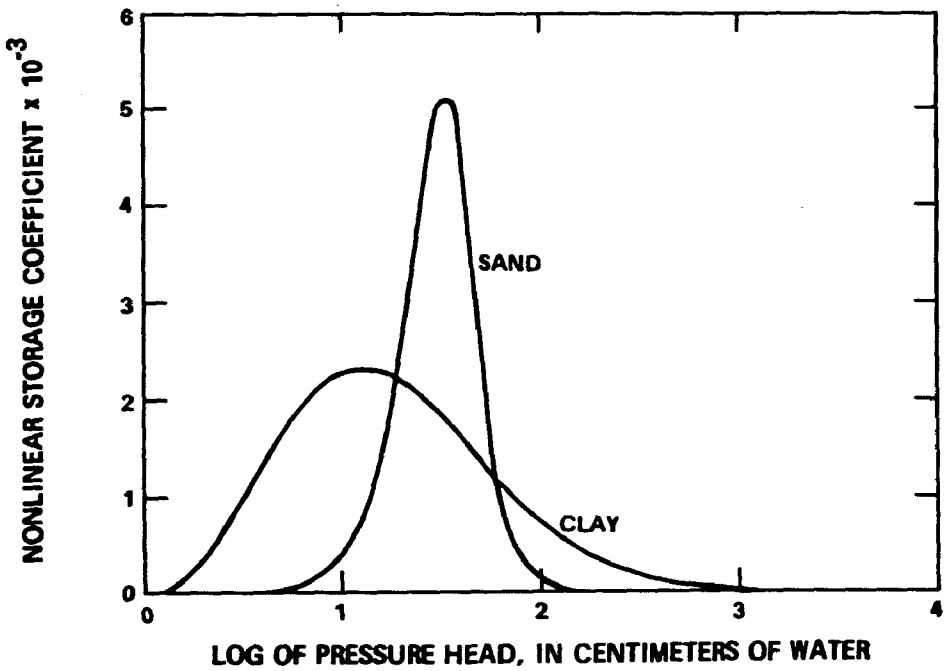

Figure 2. -- Nonlinear storage coefficient for a sand and clay.

Table 1.--*Degree of nonlinearity found in most formulations of equations 8-12*

[V = very nonlinear, S = slightly nonlinear, L = can be assumed linear]

Equation	Transport coefficients		Source and sink terms	Boundary conditions
	Storage	Dispersion, diffusion, or conductance		
(8) Liquid water----------	V	V	S-V	S-V
(9) Moist air----------	S	V	S	S
(10) Water vapor and gaseous pollutants-----	V	V	S-V	S-V
(11) Solutes in liquid water--	L	L	S	S
(12) Enthalpy----------	S	S	V	S-V

FACTORS THAT DETERMINE A MODELING APPROACH

There are several factors that determine the modeling method used to analyze a given field problem:

1. The degree of nonlinearity and hysteresis in transport coefficients, boundary conditions, and source/sink terms (see table 1);
2. Inclusion of an advection or gravity term;
3. Existence of sharp fronts;
4. Heterogeneity and anisotropy;
5. Existence of complex boundaries;
6. Data availability;
7. Time and funding available;
8. Necessity to couple two or more of equations 8-12.

Factor 8, coupling of equations, will be discussed first, with factors 1 through 7 discussed in following sections.

Equations 8-12 are all coupled to some degree. The following two examples illustrate coupling. The liquid and solute flux equations are coupled, because the liquid flux is required to evaluate the advection term in the solute flux equation. Hydraulic conductivity in the liquid flux equation may also depend on the solute concentration (as discussed previously). The thermal potential appearing in the liquid flux equation (equation 8) depends upon the temperature distribution derived from the energy flux equation (equation 12).

The degree of coupling required in solutions to the pertinent equations depends principally upon the difference in time scales in the phenomena being modeled. For example, air pressure response is generally very rapid compared to liquid response, so that implicit consideration of simultaneous air and water flow due to pressure gradients is not required unless air pockets are entrapped. Large differences in time scales may be used to advantage in solving field problems by specifying the values of a rapid response variable as boundary conditions for a variable that responds less rapidly. Sometimes the sensitivity to time variations in a secondary variable in an equation is low with respect to the response of the principle variable. For example, it has been shown by Wierenga (1977) and Beese and Wierenga (1980) that, under certain conditions, the pollutant concentration at depth in a soil profile can be simulated as well using a time-averaged water-flux rate ($\bar{q}_f$) (in equation 11), as with a fully transient treatment yielding the time variations in q_f that are caused by cyclic variations in rainfall and evaporation.

When it is required to couple two or more of equations 8-12 for a given application, care must be taken in proper boundary-condition specifications with respect to all coupled equations.

Coupled equations are complex enough to generally preclude any analytical or quasi-analytical approach. The numeric methods couple the equations by either solving them sequentially or simultaneously. Coupling of equations using a sequential solution is usually accomplished through the use of source and sink terms. For example, in a problem of combined heat and liquid flow (equations 8 and 12), the liquid movement due to thermal gradients is incorporated as a source or sink in equation 8, and the movement of heat by moving fluid may be incorporated as a sink in the enthalpy flux equation (equation 12). Sequential solutions are exemplified by water and solute flow problems where the water flow equation (equation 8) is solved first, and the resultant fluid velocities are used in the solute flow equation (equation 11). If the degree of coupling is slight, this two-step sequential procedure is generally adequate. For strongly coupled problems such as coupled heat and moisture flow problems, however, the solutions from the two-step process must be improved by iteration. This iteration can be accomplished either separately or combined with the iteration required to linearize nonlinear forms of the equations, and the iteration that may be used to solve the linearized algebraic equations. Table 2 summarizes the degree of coupling of equations 8-12 for most problems relative to waste-disposal studies.

Table 2.--*Degree of coupling of equations 8-12 exhibited in problems relating to radioactive waste disposal*

[S = strongly coupled, M = moderately coupled, W = weakly coupled]

Equation	Equation number 9	10	11	12
	Moist air	Water vapor and gaseous pollutants	Solute dissolved in liquid	Enthalpy
(8) Liquid water----------	M	W-M	S	M-S
(9) Moist air----------	---	W-M	W	M
(10) Water vapor and gaseous pollutants--	---	---	M	S
(11) Solute dissolved in liquid----------	---	---	---	W-M

Analytic and Quasi-analytic Methods

When the problem to be solved can be cast in simple form, a closed form analytic or quasi-analytic method may be available. These can be classified as direct, similarity, quasilinear, and integral methods.

These categories are attributed to a review by Philip (1974). The discussion that follows is written with emphasis on solutions to the nonlinear form of equation 8, the water-flow problem. However, the methods apply equally well to nonlinear forms of equations 9-12. Analytic solution methods for linear forms of equations 8-12 will not be explicitly addressed in this paper; solutions to linear problems are, in general, special cases of the nonlinear methods presented. A review of analytic solutions to the solute flux equation (equation 11) will be given by another paper at this symposium (Grove and Kipp, 1980).

Direct Methods

Direct methods involve direct integration of some form of the descriptive equation, solving for the constants of integration using boundary and initial conditions. A simple example would be the problem of isothermal isohaline steady upward flux from a shallow water table at a depth ℓ. The governing equation is Darcy's law (equation 3), because the time derivative appearing in equation 8 is zero. If the desired flux rate is q, then the problem can be written as:

$$\ell = \int_{\psi_{z=\ell}}^{\psi_{z=0}} \frac{K(\psi)}{q + K(\psi)} \, d\psi, \tag{14}$$

which for certain analytic forms of $K(\psi)$ can be integrated directly. Gardner (1958, 1959) and Ripple and others (1970) detail this solution method for both uniform and layered media. The integral in equation 14 may not be integrable in closed form because of the nature of the $K(\psi)$ function. In this case, numerical integration methods such as Gaussian quadrature must be used, but this solution type can still be termed a direct method. An application of direct solution methods that is important in transient infiltration problems is the assumption of a step function shape for the wetting front. This has been shown to be equivalent to the assumption to a step function for hydraulic diffusivity, $D = K/S$ (Philip, 1973). The resultant formulation, which is attributed to Green and Ampt (1911), has been shown to accurately represent the infiltration rate under conditions of ponded water on the surface. Mein and Larson (1973) have extended the method to a flux boundary condition imposed by constant rainfall rates.

Direct integration methods require the descriptive equation to be a function of only one independent variable; thus, transient problems are not immediately amenable to this solution method. However, the use of a similarity variable that combines two independent variables may render the problem tractable by direct methods. The most common of these transformations is the so-called Boltzman transformation (Ames, 1965):

$$\phi = xt^{-\frac{1}{2}} \tag{15}$$

where

ϕ is the transformed variable,
x is a spatial coordinate, and
t is time.

Even though a similarity transformation reduces the number of independent variables by one, direct solution still requires the transport coefficients to be constants or to have simple linear or step function dependence on the transformed independent variable.

Linearization

When the transport coefficients cannot be expressed as simple functions the descriptive equations must be linearized. The most common linearization method used in the reviewed reports consists of using an exponential function to describe hydraulic conductivity for steady-flow problems, and hydraulic diffusivity (D) for transient problems.

The exponential dependence of hydraulic conductivity on pressure potential for example can be described by

$$K = K_s \exp(\alpha \psi) \tag{16}$$

where

K_s = the hydraulic conductivity at saturation, and

α = a constant.

The second step in the linearization process is to introduce a new variable termed the matric flux potential, by using the Kirchoff transformation (Ames, 1965):

$$\nu = \int_{\psi_o}^{\psi} K(a)\, da \tag{17}$$

These steps result in a linear form of equation 8 written with ν as the dependent variable, and render essentially all steady-flow problems solvable using linear methods (Philip, 1974). It should be noted that for a wide range of soils, the $K(\psi)$ function is very well represented by equation 16 (Laliberte and others, 1966; Mualem, 1976).

Approximate Analytic Methods

When a linearized form of the descriptive equations cannot be solved by direct integration, approximate methods must be used. These can be categorized as series expansion methods and integral methods. Series expansion methods involve expressing the solution as a series with unknown coefficients that usually involve integrals of the transport coefficients. The form of the series is often based on empirical observation. Philip (1955) was the first to apply this method of solution to nonlinear equations described by equation 8. Philip's solution is of the form:

$$X = \phi t^{\frac{1}{2}} + \chi t + \omega t^{3/2} + \ldots \qquad (18)$$

where ϕ, χ, ω, are the unknown coefficients. The expansion in terms of $t^{\frac{1}{2}}$ is based upon the observed square root of time dependence of the advance of a wetting front in the absence of gravity. The coefficients in equation 18 can be determined by an iterative trial and error process proposed by Philip for arbitrary forms of the transport coefficients. When this process is followed, the method is essentially a numerical rather than an analytic method. Brutsaert (1968a, b, 1977) has derived exact expressions for the first two coefficients in the above equation for one-dimensional absorption (gravitational potential ignored), and infiltration (gravitational potential included), by using a flux potential formulation and assuming a simple form for the nonlinear storage coefficient. The principal drawback to Philip's method is its divergence from the true solution at long times. The maximum applicable time may be a few days or less (Brutsaert, 1977).

Series solutions may also be derived by expressing the series in terms of a perturbation variable, or some variable that is assumed to vary a small amount over the range of the solution (Ames, 1965). Babu (1976a, b, c, and 1977), has used this solution method, with the terms in the series involving integrals of the hydraulic diffusivity function.

The other general category of approximate analytic methods that can be applied to transient as well as steady-state problems involves an iterative evaluation of an integral form of equation 8. The method is useful in reducing the number of independent variables in problems that cannot meet the similarity requirements (Philip, 1974). The method involves making a first approximation to the form of the solution to equation 8. This may be accomplished by ignoring the time-dependent first term and solving the resultant steady-state problem by use of the previously discussed methods. This first approximation is inserted in the integral of the transient equation with respect to the variable to be eliminated. The resultant equation is solved by a direct or series solution method.

These steps may be repeated to iteratively improve the solution. Ames (1965) gives a further explanation of these iterative methods.

Parlange, in a series of papers (1971a, b, c; 1972a, b, c; 1973a) has applied the iterative method to a variety of problems ranging from one-dimensional transient absorption to axisymetric transient infiltration problems. Cisler (1974) derived a correction to Parlange's method which improved the accuracy significantly. These iterative methods are very sensitive to the initial estimate of the solution. Knight and Philip (1973) have shown that these methods can fail to converge if the initial estimate is very far from the solution. Parlange and Braddock (1978) have shown that iterative methods may converge to the wrong solution after a finite number of iterations.

Availability of Analytic Solutions

The length restrictions for a symposium paper preclude listing all the analytic solutions found in this review. An excellent compilation of the available solutions through 1971 is given by Braester and others (1971). Solutions since 1971 are summarized in Babu (1976a, b, c, and 1977); Philip (1974); Parlange and Babu (1976a, b); Raats (1971, 1972, and 1977); Lomen and Warrick (1976a, b, and 1978a, b); Warrick (1974); and Warrick and Lomen (1977). A summary of the types of problems that have been solved for the nonlinear water flow equation is given in table 3. One-dimensional problems have been solved for a variety of realistic boundary conditions. The principal restrictions are: (1) The requirement to use simple forms for the functional dependence of the transport coefficients upon the solution variable; (2) the limiting of heterogeneous media in transient cases to simple functional dependence upon depth; and (3) the failure to include source and sink terms of a general nature.

For multidimensional cases, the geometry is restricted to two-dimensional planar and three-dimensional cylindrical or spherical symmetry. Few transient multidimensional problems have been analyzed, and no solutions to multidimensional transient problems that involve sources and sinks were found.

While it may appear that the application of analytic solutions to field problems that relate to waste disposal is somewhat limited, there are three main advantages to these methods. First, they give closed-form solutions that allow general conclusions to be drawn regarding the movement of mass and (or) energy in variably saturated systems. Second, these conclusions can be used in a qualitative sense to check the results of approximate numeric methods. Third, analytic solutions that exist for simple problems can be used quantitatively to check approximate numeric methods applied to the same simple problems. Examples of these generalities are the square root of time dependence of horizontal absorption and the initial stages of vertical infiltration, and acceptable forms of moisture and potential profiles for simple systems (Childs, 1969).

Table 3.--*Types of variably saturated flow problems for which analytic and quasi-analytic solutions are available*

Factor	Number of reported solutions			
	One-dimensional		Two and three-dimensional	
	Steady	Transient	Steady	Transient
No gravity term:				
Homogeneous:				
Source/sink-------	1	0	0	0
No source/sink----	1	24	0	5
Heterogeneous:				
Source/sink-------	0	0	0	0
No source/sink----	0	0	0	0
Gravity term:				
Homogeneous:				
Source/sink-------	2	1	3	1
No source/sink----	2	21	11	3
Heterogeneous:				
Source/sink-------	0	0	0	0
No source/sink----	4	2	2	0

Numeric Methods

Numeric methods require subdividing the spatial and temporal domains into discrete intervals over which the variables such as pressure, temperature and concentration are assumed to be either constant or to vary in a simple manner. This discretization results in a set of non-linear algebraic equations that must first be linearized and then solved simultaneously, usually using high-speed digital computers.

The emphasis of the following discussion is on solutions to the liquid flow equation (equation 8); however, the methods are applicable to nonlinear forms of any of equations 8-12.

The principal advantage of numeric methods is their flexibility. In principle, methods that are suitable for one dimension can be simply extended to two and three dimensions. Conversely, computer codes incorporating these methods for multi-dimensional problems can collapse to handle one-dimensional cases. Complex boundaries, nonlinear transport coefficients and boundary conditions, heterogeneity and anisotropy, and spatial and temporal source/sink variations can all be handled. The principal disadvantages of numeric methods for nonlinear problems are the large computer core and time requirements and the complexity of computer codes.

The following discussion is pertinent to the solution of the water flow equation. By suitable rearrangement, this equation can be written in terms of one of three variables. If the system under consideration remains unsaturated at all times, the flow equation can be written in terms of the volumetric moisture content (θ). This is referred to as the 'θ-based' approach, in which the driving forces are gradients in moisture-content concentration. The θ-based equation is identical in appearance with the solute-flux equation (equation 11), with the gravity-driven flux term in equation 8 being equivalent to the advective term in equation 11. When part of the system is saturated, this approach fails, because the volumetric moisture content remains constant at saturation, but flow still occurs due to gradients in pressure, gravitational, and thermal potentials. For partially saturated systems, equation 8 can be written in terms of the matric flux potential (equation 17), the pressure potential ϕ_p, or the sum of the pressure and gravitational potentials $(\phi_p + \phi_g)$. The pressure-potential approach can also be referred to as the pressure-head (h) approach by using units of length for the pressure potential: $h = \frac{\phi_p}{\rho g}$, where g = gravitational acceleration. Similarly, the combined pressure and gravitational potential approach is often termed the total head (H) approach, where $H = \frac{1}{\rho g}(\phi_p + \phi_z) = (h + z)$, where z is the height above an arbitrary datum. These two approaches have the advantage that h or H is continuous, whether the system is saturated or not. In this case, boundaries between saturated and unsaturated zones are surfaces where h = 0, with h being positive in the saturated, and negative in the unsaturated zones.

Spatial Discretization Methods

There are two basic methods of subdividing the spatial domain of a problem described by equations 8-12: the use of finite differences or finite elements.

Finite-difference methods require subdivision of the region considered into subregions that have a regular geometry. These regions are usually rectangular, but arbitrary polygonal subregions have also been used (Narasimhan and Witherspoon, 1977). In finite-difference methods, spatial derivatives are approximated by assuming that the solution variable varies linearly between the geometric centers of each of the subregions, and the storage coefficients are assumed to be constant over each subregion. Any sources or sinks present are assumed to contribute uniformly over each subregion in which they are present.

Because the gradients in the solution variable are assumed to be linear between adjacent subregions, the use of finite-difference methods may require many subdivisions in problems that involve rapidly changing gradients; many problems in variably saturated flow described by equations 8-12 are this type. Examples are wetting fronts in infiltration problems; sharp solute concentration fronts resulting from a step or pulse input of contaminant; and evaporation-condensation fronts in combined heat and moisture flow from a buried heat source. The existence of sharp fronts can result in oscillatory solutions even if a fine grid spacing is used (Finlayson and others, 1978). For these types of problems, a numerical dispersion term is often added. For the water-flow problem, the use of upstream weighting on relative hydraulic conductivity is commonly used (Brutsaert, 1971; Finlayson and others, 1978). Similar terms must often be used in finite difference solutions to equations with a strong advection term (equations 11 and 12) to prevent oscillations.

The requirement for fine subdivision to accurately represent sharp fronts may result in a large number of simultaneous equations that must be solved. This restriction, when combined with restrictions on time-step length to prevent oscillation and nonconvergence caused by nonlinearities and (or) presence of an advection term, can result in formulations of field problems that are very expensive to solve.

Another disadvantage of finite-difference methods is that, due to the regular shape of the subregions, many subregions may be required to accurately represent the geometry of a given field problem.

Accurate representation of complex geometries is an advantage of the finite-element method of spatial discretization. In this method, the region of interest is subdivided into subregions or elements that may have irregular shapes. These may be simple linear quadralaterals, triangles, or complex quadralaterals with curved sides.

In solving the balance equations 8-12 for these irregular subregions with a finite-element method, the surface integrals are converted to volume integrals using Gauss' divergence theorem. The resultant equations are evaluated at a finite number of points or nodes that coincide with the vertices of and points interior to the subregions or elements. For example, the solute transport equation (equation 10) would become:

$$\varepsilon = S_c \frac{\partial \hat{\rho}_c}{\partial t} + \nabla(q_f \hat{\rho}_c) - \nabla \cdot L \nabla \hat{\rho}_c . \qquad (19)$$

where

ε is a residual between the approximate and true solutions, and

$\hat{\rho}_c$ is the approximate value of ρ_c.

There are two types of finite element methods: those derived using variational calculus, and those based on the method of weighted residuals. Only the latter will be discussed in this paper as most of the published solutions to equations 8-12 use them, and because the resultant equations from both methods are the same in cases where a variational formulation exists.

The weighted-residual methods multiply the residual, ε, by a weighting function, which is a polynomial in the spatial coordinates only. To minimize the error of approximation, it is then required that:

$$\int_V \varepsilon w_i \, dV = 0, \quad i = 1, \ldots . m \qquad (20)$$

where there are m weighting functions over the solution domain. This step in the finite-element method results in a powerful tool to control the accuracy of the approximate solution by choosing suitable weighting functions (w_i). This has been an important advance in simulating some sharp front problems (Bender and others, 1975).

The next step in weighted-residual finite-element methods is to approximate the solution variable with a series of the form:

$$h \simeq \sum_{j=1}^{M} \hat{h}_j (t) \, \omega_j (x) \qquad (21)$$

where

$\hat{h}_j$ (t) is an unknown coefficient which becomes the desired solution variable, and

ω_j (x) are basis functions that are a function of space only.

The choice of basis functions defines further the type of finite-element method used. If the basis functions are chosen to be the same as the weighting functions (w_i in equation 20), then the method is a Galerkin method (Finlayson and others, 1978). If the basis functions are chosen to be proportional to dirac delta functions, then the method is an orthogonal collocation method (Finlayson and others, 1978).

Galerkin methods applied to forms of equations 8-12 that include a nonlinear storage term can result in oscillations when sharp fronts are involved (Mercer and Faust, 1977). Since the solution of the algebraic

equations resulting from either finite-difference or finite-element methods often requires iteration due to nonlinearity of the problem, these oscillations very often result in a failure of the iterative process to converge. The oscillations are caused by the evaluation of the nonlinear storage term at points adjacent to the point of interest. These oscillations can be minimized by a Galerkin formulation that evaluates the storage terms as an integrated average over each element (Neuman, 1973). This is sometimes called capacitance lumping. Orthogonal collocation on finite elements results in a formulation that does not include the extra storage terms, and hence, is free of this type of oscillations (Finlayson and others, 1978).

The following conclusions regarding the preferability of finite-difference or finite-element methods are adapted from Finlayson and others (1978, p. 72) in a study of numerical methods applied to very dry soils.

1. "***finite elements*** (Galerkin and orthogonal collocation)*** are capable of tracking steeper fronts than finite difference methods***."
2. Most predictive simulations in hydrology using finite element methods have not involved fronts as steep as those encountered in infiltration into extremely dry soils.
3. "***for linear problems with steep fronts, finite element methods are much faster for equivalent accuracy (than finite difference methods). For nonlinear problems, the Galerkin finite element methods are slower than finite difference methods***."
4. "***for both finite difference and finite element methods,*** very steep fronts can only be handled by including numerical dispersion in the form of averaged (or upstream)(conductivities), special weighting functions or some other techniques***" "***As the front becomes steeper, the number of spatial nodes or grid points increases and the time step (required to minimize oscillations) correspondingly decreases***."
5. "***The preferred method for dry soils is a finite difference method with averaged (conductivities) because it introduces numerical dispersion and allows calculations without a prohibitively large number of nodes***."

Time Integration Schemes

Once the spatial derivatives in equations 8-12 have been approximated by either a finite-difference or finite-element scheme, time derivatives must be approximated in some fashion. For both finite-difference and finite-element spatial discretizations, this is usually done using finite differences in time. It is possible to use the Galerkin approximation (similar to equation 21) for the time derivative, as described by Gray and Pinder (1974) and Zyvoloski (1973). However, it has been shown that no significant accuracy improvement is obtained by this method and that additional computation is required to formulate and solve the resulting algebraic equations (Yoon and Yeh, 1975).

Commonly used time-differencing schemes evaluate the spatial derivative approximations at the previous time-step (explicit method), the current time-step (implicit method) or as a weighted average of these (Crank-Nicolson method). The explicit method results in the simplest set of equations to solve, but is subject to stability restrictions on the step length that often make its use infeasible (Haverkamp and others, 1977). The Crank-Nicholson method is the most accurate, but Jeppson (1974a) has shown that, if the nonlinear transport coefficients are used with a Crank-Nicholson method that is valid for constant coefficients, the solution is grossly in error. If a Crank-Nicholson scheme that is valid for varying coefficients is used, Jeppson (1972) also showed that, if the storage coefficient is divided into the conductivity terms before the equations are solved, the resulting system of equations is difficult if not impossible to solve, due to rapid oscillations in the neighborhood of the true solution. In addition to these problems, Neuman (1975b) showed that a Crank-Nicholson approach cannot be used in solution of equation 8 for problems in which part of the system is saturated and boundary conditions change in the saturated zone.

The fully implicit method, which evaluates the spatial derivative approximations at the current time-step, appears to be the preferred method (Jeppson, 1974a; Neuman, 1975b; Haverkamp and others, 1977). While it is slightly less accurate than the Crank-Nicholson approximation, it permits solution of the widest range of problems likely to be encountered in waste-disposal problems.

Recently, Narasimhan and Witherspoon (1977, 1978a and b), and Narasimhan and others (1978) developed models that utilize a so-called mixed explicit-implicit time-integration scheme. This scheme is based on the following: stability criteria for explicit methods depend on the rate of change of the solution variable, being more stringent for small grid spacings and for rapid changes in the solution variable. Many problems may involve subregions over which changes are slow due to a large ratio between the storage coefficient and the conductance or to large elements or finite-difference cells. The equations for these subregions can often be evaluated explicitly, requiring implicit evaluation only where rapid changes are occurring. However, in many cases, the computer time required to evaluate the status of all points in the system may be greater than if the entire region had been evaluated implicitly.

Another time-integration scheme takes advantage of the fact that after the spatial derivatives have been approximated by finite differences or finite elements, the result is a set of ordinary differential equations of the form:

$$S \frac{dh}{dt} = \Delta_x^2 h, \tag{22}$$

where $\Delta_x^2 h$ is the approximation to the spatial derivatives. This set of equations can be integrated in time using methods developed for ordinary differential equations. The most common of these methods are fourth-order Runge-Kutta and fifth-order Milne (James and others, 1968; International Business Machines, 1975). These are essentially explicit methods and are

subject to time step restrictions. Haverkamp and others (1977) found that 5 to 10 times more computer time was required to solve the nonlinear one-dimensional water-flow problem with these methods than with a fully implicit scheme.

The principal advantage of these methods of time integration is that they have been incorporated into an applications-oriented language by International Business Machines (1975) entitled: "Continuous System Modeling Program" (CSMP). This language makes it very simple to code a model for a particular application. Hillel (1977) gives sample programs using CSMP for solving one-dimensional finite differenced forms of the water flow equation (8); water and solute flow equations (8 and 11); and moisture and heat flow equations (8, 10, and 12). CSMP solutions to equation 8 have also been reported by Van der Ploeg and others (1974) and Bhuiyan and others (1971). Combined one-dimensional solute and water-flow problems have been solved by CSMP and reported by Wierenga (1977), Beese and Wierenga (1980), and Siddle and others (1977).

Linearization Methods

Any or all of equations 8-12 may exhibit some degree of nonlinearity in the transport coefficients or boundary conditions. Since the equations resulting from any spatial and temporal discretization schemes must be linear to solve, some form of linearization is required. Three main linearization methods commonly have been used: explicit methods, predictor-corrector methods, and fully implicit methods.

Explicit linearization involves evaluation of the nonlinear coefficients and boundary conditions using values of the solution variable from the previous time step. As would be expected, this method may require very small time steps to achieve acceptable accuracy (Jeppson, 1974a; Rubin, 1968; Haverkamp and others, 1977). For infiltration problems, the general effect of explicit linearization with large time steps is for the solution to lag behind the true solution (Haverkamp and others, 1977).

Predictor-corrector methods involve two iterations for each time step. The first step solves the equations for one-half the step length using the coefficients evaluated at the previous time step or by extrapolating to one-half the time step. Extrapolation may use the previous two or three time steps (Rubin, 1967). The solution is then repeated for the full time step, using the values of the solution variable at one-half the time step to evaluate the coefficients. Jeppson (1974a) has shown that oscillations in sharp fronts can result from this method. The accuracy of the method is dependent on the accuracy of the extrapolation; since iteration is not continued until convergence, instability can result (Jeppson, 1974a; Braester and others, 1971), particularly with highly nonlinear problems.

Fully implicit schemes involve evaluating the nonlinear coefficients and boundary conditions at the current time step by iteratively solving the equations until convergence occurs. The value of the solution variable to evaluate the coefficient for the first iteration may be obtained by extrapolation from previous time steps (Freeze, 1971b; Neuman, 1975b). While implicit linearization may be the most time-consuming method, it results in the most stable, accurate scheme with the least computational effort (Haverkamp and others, 1977). In addition, the iterative process gives a means of controlling the accuracy of the solution by specifying the convergence tolerance.

Although all numeric schemes require a large number of computations, iterative linearization requires an even larger number. This would be only of passing interest, except the earliest reference this author found to the solution of a form of equation 8 describing vertical one-dimensional water flow was accomplished by Klute in 1952, using hand calculations for a fully implicit iterative scheme.

Convergence of fully implicit iterative linearization schemes is not guaranteed, and may be slow. The most effective means of accelerating convergence is to apply a Newton-Raphson scheme to the matrix equations (Jeppson, 1974b; Brutsaert, 1971; Mercer and Faust, 1977; Finnemore, 1970). This scheme may be applied to both the conductivity and storage terms, or to the more nonlinear of the two. This author has found it sufficient for many highly nonlinear problems to apply this linearization technique to the storage term only.

The iteration required to solve nonlinear equations often fails to converge when the solution is approached. The convergence failure takes the form of oscillations around the true solution, and often occurs when static equilibrium is approached. There is no panacea for this problem; however, the use of an adjustable damping factor often will result in convergent solutions. This is an ad hoc procedure; a more rigorous approach to optimize the iterative process for nonlinear problems is currently being investigated by R. L. Cooley, U. S. Geological Survey (oral commun., 1980).

Matrix Solution Methods

All numerical schemes except those involving explicit time and coefficient evaluation result in a set of algebraic equations that must be solved simultaneously. These equations can be written in matrix form as:

$$[A]\{\frac{dh}{dt}\} + [B]\{h\} = \{r\}$$

Direct methods involve some form of Gaussian elimination and take advantage of the sparse nature of the coefficient matrices [A] and [B]. These methods generally require large computer storage and time requirements. To obtain accurate solutions, roundoff and truncation error must be minimized by the proper use of single and double-precision arithmetic,

and such features as pivoting to assure diagonal dominance of the matrices [A] and [B] (Nobel, 1969). Recent advances in equation ordering (Price and Coats, 1973) have significantly optimized the storage and time requirements for using direct solution methods, thus making their use more feasible for large problems.

The most commonly used iterative matrix solution methods are the iterative alternating direction implicit (IADI), line successive over relaxation (LSOR), and the strongly implicit (SIP) methods. These methods solve sets of simultaneous equations by iteratively improving an initial guess at the solution. The initial guess uses values of the solution variable from the previous time step. As Braester and others (1971, p. 113) point out, "***unfortunately however, none of the methods (LSOR, IADI) will guarantee convergence of the unsaturated flow solution in all cases***."

It should be noted that if the matrix equations are solved by an iterative procedure, this procedure must be embedded in the iteration required to handle the nonlinearity of the equations. Some authors (Freeze, 1971; Brutsaert, 1971) have accomplished this requirement with an "inner iteration loop" to solve the matrix equations and an "outer iteration loop" to handle the nonlinearity. This author and others have found it efficient to combine the two iterative loops.

The principal advantages of iterative-solution methods over direct methods are: (1) smaller computer core requirements; and (2) ability to control the accuracy of the solution (and hence its cost) by specifying the convergence criteria. For example, this author has found it computationally more efficient to solve strongly nonlinear problems to the same degree of accuracy with LSOR with a very restrictive convergence criteria rather than a direct solution with a less stringent criteria.

Availability of Verified Numeric Models

Over 280 references to numeric solutions to nonlinear forms of equations 8-12 were found in the literature. The earliest solutions were for simple one-dimensional liquid-water absorption problems. Present capability includes solutions of complex three-dimensional water and solute-flow problems and coupled-heat and moisture-flow problems. Figures 3 through 6 summarize chronological development of models incorporating these solutions.

Although many real-world problems can be solved by making the one-dimensional approximation to the required equations, general codes should have multidimensional capabilities. Many of these codes have been applied to a variety of field problems. Table 4 lists the capabilities, applications, and limitations of using some of these codes. While the codes in table 4 are documented and verified, their use is not necessarily straightforward because of the many numerical tricks that may be required to obtain a solution. Extreme nonlinearities can preclude solutions in many cases. These problems are inherent to the nature of the nonlinear

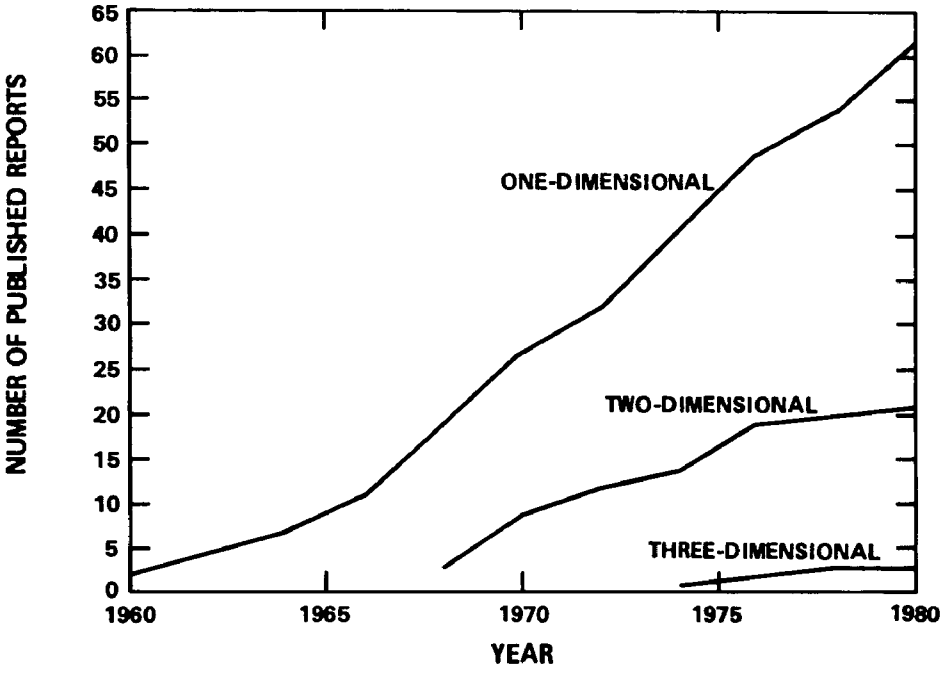

Figure 3. -- Development of variably saturated finite difference models since 1960.

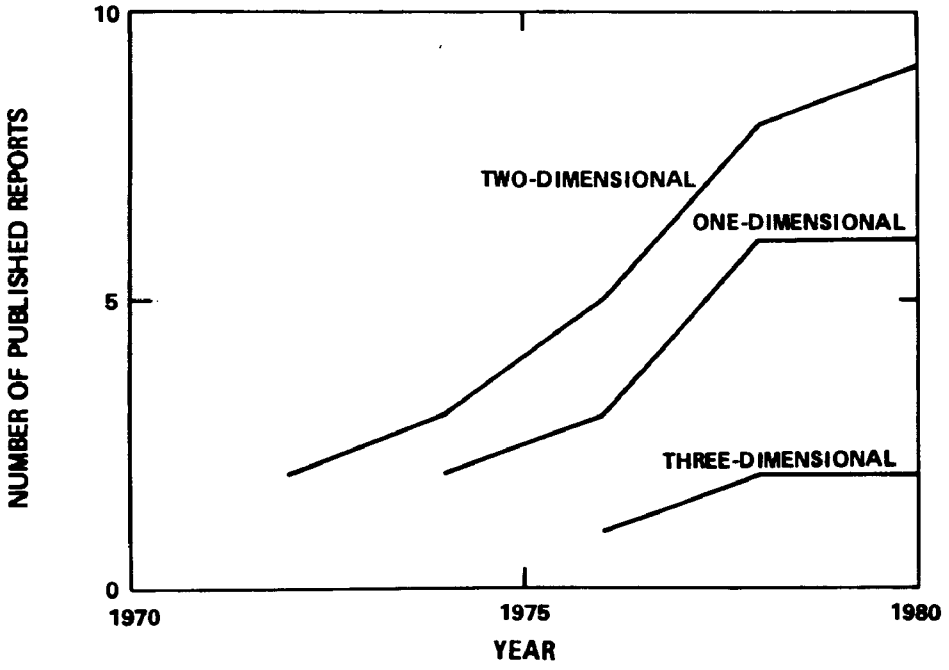

Figure 4. -- Development of variably saturated finite element models since 1970.

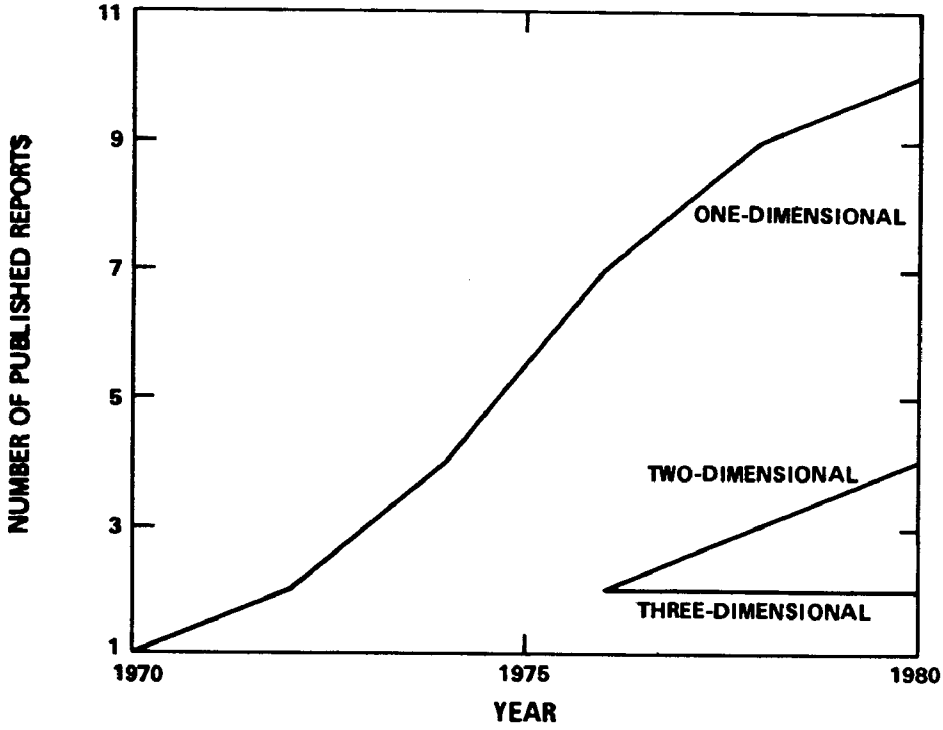

Figure 5. -- Development of variably saturated water and solute transport models since 1970.

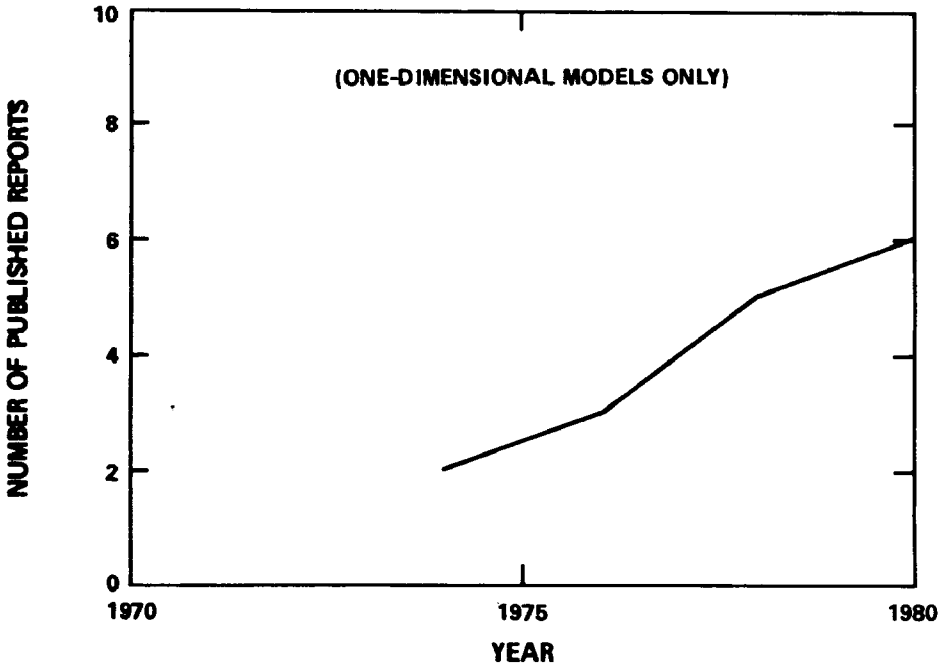

Figure 6. -- Development of variably saturated water and heat transport models since 1970.

Table 4.--*Features of available general computer codes for numeric solution of variably saturated water, solute, and heat transport problems relating to radioactive waste disposal*

Model name	Authors	Maximum dimensions	Solute transport	Heat transport	Spatial discretization	Time integration	Linearization	Solution	Source/sink types	Boundary condition types	Verification	Remarks
	Baca, King, and Norton (1973)	1	No	Yes	Galerkin-finite element	Implicit	Implicit with Newton-Raphson	Gaussian elimination	Explicit	All	Field data, isothermal column data, analytic solution	Log transformation of pressure head - unsaturated conditions only
	Brandt and others (1971)	2 (3-axisymmetric)	No	No	Finite difference		Implicit with Newton-Raphson	ADI	None	All	Unknown	θ-based - unsaturated conditions only
	Bresler (1975)	2 (3-axisymmetric)	Yes	No	Finite difference	Crank-Nicholson	Implicit with Newton-Raphson	ADI	Explicit	All	Column data	Solute transport-second order finite difference scheme some oscillations in transport solution
CSU	Brutsaert (1971)	3	No	No	Finite difference	Implicit	Implicit with Newton-Raphson	Line SOR with correction	Explicit	All, including seepage faces	Lab, field data, other models	Has been applied to a wide range of problems
	Brutsaert, Breitenbach and Sunada (1970, 1971, 1973)	2 (3-axisymmetric)	No	No	Finite difference	Implicit	Implicit with Newton-Raphson	Line SOR	Explicit	All	Lab, field data, analytic solutions	Well bore calculations 2-phase
	Caussade, and others (1979)	2	No	No	Finite difference	Explicit	Alternating linear solution with nonlinear correction	None	None	All	Analytic solution	Mildly nonlinear problems tested only
	Cooley (1981)	2 (3-axisymmetric)	No	No	Orthogonal collocation on Finite elements	Implicit	Implicit	SIP	Explicit	All, including seepage faces	Lab, field data, other models	Some problems with very nonlinear problems well-bore calculations. Unpublished research model only

Table 4.--*Features of available general computer codes for numeric solution of variably saturated water, solute, and heat transport problems relating to radioactive waste disposal*--Continued

Model name	Authors	Maximum dimensions	Solute transport	Heat transport	Spatial discretization	Time integration	Linearization	Solution	Source/sink types	Boundary condition types	Verification	Remarks
	Finlayson, Nelson, and Baca (1978)	1	No	Yes	Finite difference	Implicit	Implicit with Newton-Raphson	Unknown	Explicit	All	Field data	Temperature equation solved analytically-heat conduction only
	Freeze (1971)	3	No	No	Finite difference	Implicit	Implicit with extrapolation	Line SOR	Explicit	All, including seepage faces	Lab, field data, analytic solutions	Automatic time step control, hysteresis
	Frind, Gillham, and Pickens (1977)	3	No	No	Galerkin-finite element with lumped capacitance	Implicit	Implicit with functional expansion in space and time extrapolation	Gaussian elimination	None	All	One-dimension column drainage data	Gravity term treated explicitly, waste disposal application simulated
	Frind and Verge (1978)	3	No	No	Galerkin-finite element with lumped capacitance	Implicit	Implicit with functional expansion in space and time extrapolation	Gaussian elimination	Explicit	All	Column data, Finite difference solutions	Application to radioactive waste management area
	Hammel (1979)	1	No	Yes	Finite difference	Crank-Nicholson	Implicit	Gaussian elimination	Explicit	All	Lab and field data	
	Khaleel and Reddell (1976)	3	Yes	No	Finite difference	Implicit	Implicit	Gaussian elimination	Explicit	All	Analytic and numeric solutions, experimental data	Transport solved by method of characteristics, 2-phase air-water treatment
	Leppala (1981)	2 (3-axisymmetric)	No	No	Finite difference	Implicit	Explicit or Implicit with full or partial Newton - Raphson	LSOR, SIP, Gaussian elimination	Explicit plus extraction by roots	All	Other models, analytic solutions	Unpublished research model

Table 4.--*Features of available general computer codes for numeric solution of variably saturated water, solute, and heat transport problems relating to radioactive waste disposal*--Continued

Model name	Authors	Maximum dimensions	Solute transport	Heat transport	Spatial discretization	Time integration	Linearization	Solution	Source/sink types	Boundary condition types	Verification	Remarks
	Lappala and Pollack (1981)	2 (3-axisymmetric)	No	Yes	Finite difference	Implicit	Implicit with Newton-Raphson	LSOR, SIP, Gaussian elimination	Explicit plus roots and evaporation	All	Analytic solutions lab data	Unpublished research model
	Marino (1978)	2	Yes	No	Galerkin-finite element with lumped capacitance	Implicit	Implicit with functional expansion in space and extrapolation in time	Gaussian elimination	Explicit	All, including seepage faces	Unknown	
TRUST	Narasimhan (1975)	2 (3-axisymmetric)	No	No	Integrated finite difference	Mixed explicit-implicit	Explicit or implicit with extrapolation	Point SOR	Explicit	All	other models, analytic solutions	Hysteresis, automatic time step control, deformable media, may be slow
	Natur, King and Jeppson (1975)	2	No	No	Finite difference	Time centered	Implicit with Newton-Raphson	Point SOR	None	All	Field experimental data	Sloping coordinates
FLUMP	Neuman and Narasimhan (1977)	2 (3-axisymmetric)	No	No	Galerkin-finite element with lumped capacitance	Mixed explicit-implicit, implicit-explicit, or time centered	Implicit or explicit	Point SOR	Explicit	All	Experimental data, analytic solutions, other models	Automatic time step control, may be slow
UNSAT 2	Neuman (1972, 1973 1974, 1975)	2 (3-axisymmetric)	No	No	Galerkin-finite element with lumped capacitance	Implicit or time centered	Implicit with extrapolation	Gaussian elimination	Roots, evaporation, implicit	All, including seepage faces	Lab, field data, other numeric models, analytic solutions	User oriented, no reported application to very dry soils, well bore calculations
	Ferrens (1977)	2	No	No	Finite difference	Time centered	Implicit	IADI	Explicit	All	Unknown	Hysteresis

Table 4.--*Features of available general computer codes for numeric solution of variably saturated water, solute, and heat transport problems relating to radioactive waste disposal*--Continued

Model name	Authors	Maximum dimensions	Solute transport	Heat transport	Spatial discretization	Time integration	Linearization	Solution	Source/sink types	Boundary condition types	Verification	Remarks
	Pickens, Gillham, and Cameron (1979)	2	Yes	No	Galerkin-finite element with lumped capacitance	Implicit	Implicit with functional expansion in space and time extrapolation	Gaussian elimination	None	All, including seepage faces	Column data, finite difference models, analytic solutions	
	Reeves and Duguid (1975, 1976)	2	Yes	No	Galerkin-finite element	Implicit explicit or time centered	Implicit	Gaussian elimination	Explicit	All, including seepage faces	Finite difference models, field data	Some reports of no obtainable solution for very nonlinear problems
	Segol (1976)	3	Yes	No	Galerkin-finite element	Implicit	Implicit with extrapolation	Gaussian elimination	Explicit	All	one-dimension column, lab data, Breslers finite difference model	
	Selim and Kirkham (1973)	2	No	No	Finite difference	Implicit	Explicit	ADI	Explicit	All	Unknown	
	Taylor and Luthin (1969)	2 (3-axisymmetric)	No	No	Finite difference	Implicit	Implicit	None	None	All, including seepage faces	Lab tank data	
	Todsen (1973)	2	No	No	Finite difference	Implicit	Implicit with Newton-Raphson	SOR	Explicit	All	Unknown	Convergence problems for very nonlinear problems
	Van der Ploeg and Benecke (1974)	3	No	No		Explicit (CSMP)	Explicit	None	Explicit	All	Other models, analytic solutions	θ-based - unsaturated conditions only, No gravity term, very long CPU times

Table 4.--*Features of available general computer codes for numeric solution of variably saturated water, solute, and heat transport problems relating to radioactive waste disposal*--Continued

Model name	Authors	Maximum dimensions	Solute transport	Heat transport	Spatial discretization	Time integration	Linearization	Solution	Source/sink types	Boundary condition types	Verification	Remarks
	Vauclin and others (1975)	2	No	No	Finite difference	Implicit	Implicit	IADI	None	All, including seepage faces	Lab tank data	
	Wei and Jeppson (1971)	2 (3-axisymmetric)	No	No	Finite difference	Steady state	Newton-Raphson	SOR	None	Dirichlet	None reported	Inverse formulation in terms of potential and stream functions, Grid subdivision algorithm included
	Zyvoloski and Bruch (1973)	2	No	No	Galerkin-finite element	Time centered	Implicit with shape function expansion in space	Gaussian elimination	None	All	Finite difference models	θ-based unsaturated conditions only, long computation times

forms of equations 8-12 and the methods of numeric approximation used for their solution. A thorough understanding of the physical phenomena described by the equations themselves, the numeric methods involved, and the definitions of valid solutions (in a qualitative or semi-quantitative sense) are requisite for the responsible use of these models.

One check of the validity of numerical solutions, when the results cannot be anticipated a priori, was suggested by the National Academy of Sciences in a report on risk assessment in radioactive waste disposal studies (National Academy of Sciences, 1979). Their suggestion was the application of several models to the same problem to give a consistency check. This check is necessary because of uncertainties in a numerical model owing to roundoff and convergence errors as well as uncertainties in material properties and transport coefficients for a given field problem. Such duplicate simulation might be an affront to the authors of particular computer codes, and might appear a duplication of effort to some involved in the management of scientific studies. However, in the light of the stakes involved in proper selection and management of disposal sites for extremely hazardous wastes for very long times, such checking seems mandatory.

Parametric Models

The use of solutions to equations 8-12 discussed above depends upon several factors: (1) the availability of an analytic solution or computer code using a particular numerical solution; (2) the availability of measured values of the nonlinear transport coefficients as a function of the solution variable as well as a function of space; (3) the availability of data to calibrate the models over the range of expected conditions during the life of the disposal site; and (4) funding to adequately simulate nonlinear transport processes over periods that may exceed 1,000 years. Restrictions imposed by the last three factors may preclude the use of detailed physics-based models. In these cases, adequate predictive capability may be met by the use of parametric or input-output models.

Parametric models simulate the movement of mass or energy by considering the modeled system to consist of a series of empirical functions that transform an input into an output:

Input	→	Transfer functions	→	Output
(for example, rainfall)				(for example, infiltration rate)

Transfer functions may be purely empirical or based on some physical principle. Often, transfer functions are derived from analytic solutions to simple formulations of one part of the simulated system. As an example, the translation of rainfall into infiltration can be accomplished by using the Green-Ampt infiltration equation (see p. 19) as the transfer function.

Parametric models are most applicable to systems in which the physical and chemical processes simulated are so weakly coupled that they can be considered independent. However, some feedback mechanisms can be incorporated in these models to allow some degree of coupling.

Eagleson, in a series of papers (1978a, b, c, d, e, f, and g) gives a comprehensive overview of parametric models applied to rainfall-infiltration-runoff modeling. Comprehensive parametric models that include the movement of water in variably saturated soils are described by Skaggs (1978), Afonda (1978), Crow and others (1977), Fitzpatric and Nix (1969), Neibling (1976), and Neibling and others (1977),

Parametric models of solute movement in variably saturated systems have been described by King and Hanks (1973), and Davidson and others (1978). Dutt and others (1972) combine a numeric solution to the liquid-water flow problem with a parametric representation of the chemical transformations for an unsaturated system.

The principal advantages of parametric models are: (1) the reduced number of dependent variables and parameters; and (2) that they are usually structured to give directly the desired output in terms of mass and energy flux rates. Most analytic or numeric methods solve for the spatial and temporal variation in pressure, concentration, or temperature. Flux rates must then be computed as an additional step. Hence, parametric models directly provide the desired fluxes with less effort than numeric models. Another advantage of parametric models is that because their mathematical structure is relatively simple, the effects of uncertainties in the input can be quantitatively related to uncertainties in the output.

Parametric models usually are given some physical basis by fitting transfer functions to observed data from field experiments; this practice often limits the generality of these models. The principal disadvantage of this approach is that data collection and analysis must be pursued over long time periods to assure an adequate model.

An approach that minimizes this expensive process consists of using detailed numeric models as the "experimental facility" rather than a field site. Once a numeric model is verified, if it is sufficiently general, it may be used cheaply to conduct numerical experiments to derive the appropriate transfer functions. An example of this use of numeric models is the work of Smith (1972) in deriving rainfall-infiltration transfer functions. This seems a particularly promising area for future work.

SUMMARY

Physics-based or deterministic models that describe mass and energy transport through variably saturated porous media can be expressed by one or more nonlinear partial differential equations. These equations are derived by combining equations for continuity of mass and energy with constitutive relationships. The latter express mass or energy flux as

proportional to a driving gradient in measurable variables, such as temperature, pressure, or concentration. The proportionality functions are defined as general transport coefficients. The equations can be nonlinear because of dependence of the transport coefficients, boundary conditions and sink strengths upon temperature, pressure, or concentration.

The most flexible formulation of the nonlinear liquid-water flow problem is obtained by writing the equation in terms of pressure or total potential rather than as a concentration-dependent problem with volumetric moisture content as the solution variable. The pressure or total potential formulation allows simple unified treatment of both saturated and unsaturated conditions.

Analytic, quasi-analytic, and numeric methods are available for solving the descriptive equations for a given waste-disposal problem. Analytic and quasi-analytic solutions are generally available for most multidimensional steady-state water-flow problems, if the hydraulic conductivity can be described by an exponential function of head or moisture content. Analytic solutions that consider heterogeneity in the transport coefficients are available if the heterogeneity is restricted to layering for one-dimensional, steady-state problems, and to linear or exponential dependence on the spatial coordinates in multidimensional transient problems. Analytic solutions that include source and sink terms that are simple functions of spatial coordinates and the solution variable are available for some simple geometries.

If the assumptions required for a particular analytic solution are reasonable for analyzing waste-disposal problems, it should be used. However, most waste-disposal problems are sufficiently complex that analytic solutions are not flexible enough to provide reasonable answers. Few, if any, analytic approaches are available when two or more coupled equations are needed.

The complexities of most waste-disposal problems can usually be handled by approximate numeric methods. These methods consist of spatial discretization, using finite differences or finite elements combined with suitable time integration, linearization, and matrix solution schemes.

For problems with very mild nonlinearities in the storage term, Galerkin finite-element methods are the most flexible. These methods are particularly accurate for tracking sharp fronts. When the storage term is more than mildly nonlinear, the Galerkin finite-element schemes must be modified by lumping the storage term over each element. Orthogonal collocation on finite elements and finite differences are the most flexible solution methods for the nonlinear transport equations. The application of upstream weighting on the conductivity that may be required to prevent numerical oscillation in some problems is more straightforward in finite-difference methods than in finite-element methods.

Time-integration schemes that are fully implicit in the solution variable are preferred for nonlinear problems, and required for the variably saturated water-flow equation, when boundary conditions change in the saturated zone. Crank-Nicholson methods are the most accurate, but a scheme that is valid for nonconstant transport coefficients must be used. Explicit time-integration schemes for nonlinear problems have such stringent time-step restrictions that their use is generally not feasible for simulating large systems over long time periods.

Linearization methods that evaluate nonlinear terms using the current values of the solution variable (implicit linearization) with iterative improvement are the most accurate and flexible. Evaluating the nonlinear terms using values of the solution variables from the previous time step, and extrapolation using previous time steps without iterative improvement, can result in erroneous solutions. Implicit Newton-Raphson linearization of the storage and (or) conductance terms often speeds convergence, and is required for a convergent solution in many extremely nonlinear problems. Ad hoc damping coefficients may have to be applied to obtain convergence in many problems as they approach steady state. The matrix equations that result from the foregoing steps can be solved by some form of direct Gaussian elimination or by an iterative scheme. Direct solution methods are the most accurate if they include matrix conditioning and the proper use of single- and double-precision arithmetic. The major disadvantage of direct methods are large computer core and time requirements. Iterative matrix solution methods require less core and often less time to achieve the same accuracy. Two additional advantages of iterative methods are: (1) accuracy of the solution can be controlled by specifying convergence criteria; and (2) the methods can be efficiently embedded in the iteration required for linearization and coupling of equations.

Documented computer codes are available to handle the following types of variably saturated transport problems relative to waste disposal:

1. Three-dimensional movement of liquid water and solutes in unfractured, heterogeneous, anisotropic media;
2. Two-dimensional planar and three-dimensional axisymmetric fully coupled movement of liquid water, moist air, water vapor, and heat in unfractured heterogeneous anisotropic media;
3. Three-dimensional uncoupled movement of liquid water, moist air, and solutes in unfractured heterogeneous, anisotropic media.

Some of the multidimensional, multiphase, multicomponent codes are so general that their application to a simple problem may be inefficient. However, several codes are available that are efficient for simpler problems. The capabilities of the most flexible documented codes are summarized in table 4.

Although there are many existing computer codes with capability to simulate many realistic problems in radioactive waste disposal, there are several areas in which considerable effort should be expended to assure adequate ability to predict the fate of radionuclides and other high-level wastes emplaced in variably saturated media. These include the following:

1. The physical mechanisms of flow of water and solutes through variably saturated, fractured, and structured media need to be incorporated in simulation models. Movement through large openings in these media dominate infiltration and solute movement.

2. The direct use of detailed physics-based models for long-term (on the order of 100 to 1,000+ years) prediction of the fate of radioactive pollutants may not be defendable on the following grounds:

a. Uncertainties in data due to spatial variation of transport properties and boundary conditions may be so large that collection of the required data for adequate simulation with a detailed model would be prohibitively expensive. This data uncertainty is further compounded by the necessity to determine many transport properties in the laboratory at a generally smaller scale from the field problem; the transferability of laboratory determined data to field conditions must be established.
b. Insufficient data are available to adequately calibrate detailed models for particular sites.
c. Computer costs for running realistic problems may be prohibitive.

The need for usable, reliable prediction tools for waste-disposal problems can perhaps be better met by the use of simplified parametric or input-output models, in which the functions that translate input into output have some physical basis. These functions can often be determined by numerical experimentation with physics-based models. The physics-based models used to train the parametric models need to be verified by simulating physical and chemical transport from controlled laboratory and small-scale field experiments.

3. For both physics-based and parametric models, the uncertainty in any prediction of the fate of pollutants should be quantified, based on all the assumptions in the model and uncertainties in the data. This area of modeling of ground-water systems is in its infancy. However, it will be required so that confidence limits can be placed on any predictive results and incorporated in risk analyses used in design and management decisions.

Whether physics-based models are used directly to simulate waste-disposal problems or used to train parametric models, their adequacy should be checked by duplicate simulation of the same problems with another model or models. This step seems mandatory in the light of the complexity of most waste-disposal problems, uncertainty in model parameters, and the necessity to use numerical tricks to obtain a solution.

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VERIFICATION OF PARTIALLY SATURATED ZONE MOISTURE MIGRATION: MODEL AND FIELD FACILITIES

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ABSTRACT

Two large field-experimental facilities, designed to evaluate moisture migration under partially saturated geohydrologic conditions, have been constructed on the Hanford Site. The function of these facilities is to monitor the rate and magnitude of moisture migration. Models have been used to simulate and predict one dimensional liquid and vapor phase water migration. Parametric data from these facilities are being used for verification of the UNSAT and MPHASE codes. To date, these models have shown only limited success in the simulation of: volumetric water content, water storage, water drainage, liquid flux and vapor flux. Continued studies will enhance the capability to simulate, predict and verify moisture migration and radionuclide transport under field conditions at the Hanford Site.

INTRODUCTION

The Hanford Site located in south central Washington state was established in December, 1942. The Site was constructed for production of nuclear defense materials. For nearly four decades, nuclear fuels fabrication plants, reactors, chemical separations and processing plants, laboratories, and waste storage and waste disposal facilities have been operated. These facilities have produced substantial quantities of low-level radioactive waste materials that have been stored or permanently inturned, i.e., disposed within the partially saturated geohydrologic system at the site. Nuclear waste materials from other defense and commercial facilities have also been sent to the Hanford Site for storage or disposal.

Low-level wastes have been released within the partially saturated geologic media of the site by several disposal methods, e.g., shallow land burial. These methods rely on the geochemical sorption of long-lived radionuclides and the attenuation of liquid- and vapor-phase flux of radionuclides in arid geohydrological environments. Theoretical investigations of radionuclide and moisture transport in partially saturated systems have suggested a potential for loss of containment and migration of radionuclides away from disposal facilities. This may result in wastes entering the biosphere. As a result, numerous laboratory and field studies have been conducted to evaluate the rate, magnitude, and consequences of radionuclide and moisture migration at the Hanford Site.

Following is a generalized review of specific numerical modeling efforts and field experimental facilities that have been used in part, for the validation of these models. The purpose of this report is to show the initial results and complexities of modeling and experimental studies to understand and verify migration of liquid- and vapor-phase materials in the geohydrologic system, relative to low-level waste disposal. The results of this report cannot be considered conclusive relative to validation of the models. Results are given only to enumerate progress toward this goal.

Much of the information reported here has been taken directly from published reports originating from the Hanford Site.

METHODS AND MATERIALS

SHALLOW CAISSON, LYSIMETER, MICROMETEOROLOGICAL FACILITY

A Shallow Caisson, Lysimeter, Micrometeorological experimental facility was constructed on the Hanford Site in 1978.[1,2,3] This facility was expressly designed for: (1) development and calibration of monitoring instruments and (2) development of methods to evaluate mass and energy balance factors that control radionuclide transport in and around shallow, partially saturated, geohydrologic systems. In addition, the Shallow Facility was designed to function analogous to a one-dimensional, shallow land, waste burial structure. Experimentation and monitoring activities were also conducted that were amenable to model validation, i.e., one-dimensional, nonisothermal, diphasic, partially saturated water and radionuclide transport.

The Shallow Facility, Figure 1, shows micrometeorological and hydrogeological monitoring instrumentation as it exists at present.

The Shallow Facility consists of three buried caissons 8.1 m by 2.7 m, and four buried caissons 7.5 m by 0.6 m. These caissons are attached to form a seven-caisson array. The caissons are interconnected with steel tubing to provide access to the outer caissons from the central caisson. These tubes are installed at 15-cm vertical intervals between the central caisson and large caissons and between the central caisson and small caissons at 30 cm intervals. The tubes provide access for instruments and destructive sampling of radiocontaminants and other materials.

Weighing lysimeters to determine mass balance are installed below grade and attached to the central caisson. Uniform sand was backfilled into the six peripheral caissons of the array between 8.1 m and 6.3 m deep. A layer of coarse quartz sand was then introduced into the caissons between 6.0 m and 6.3 m. This layer provided for evaluation of

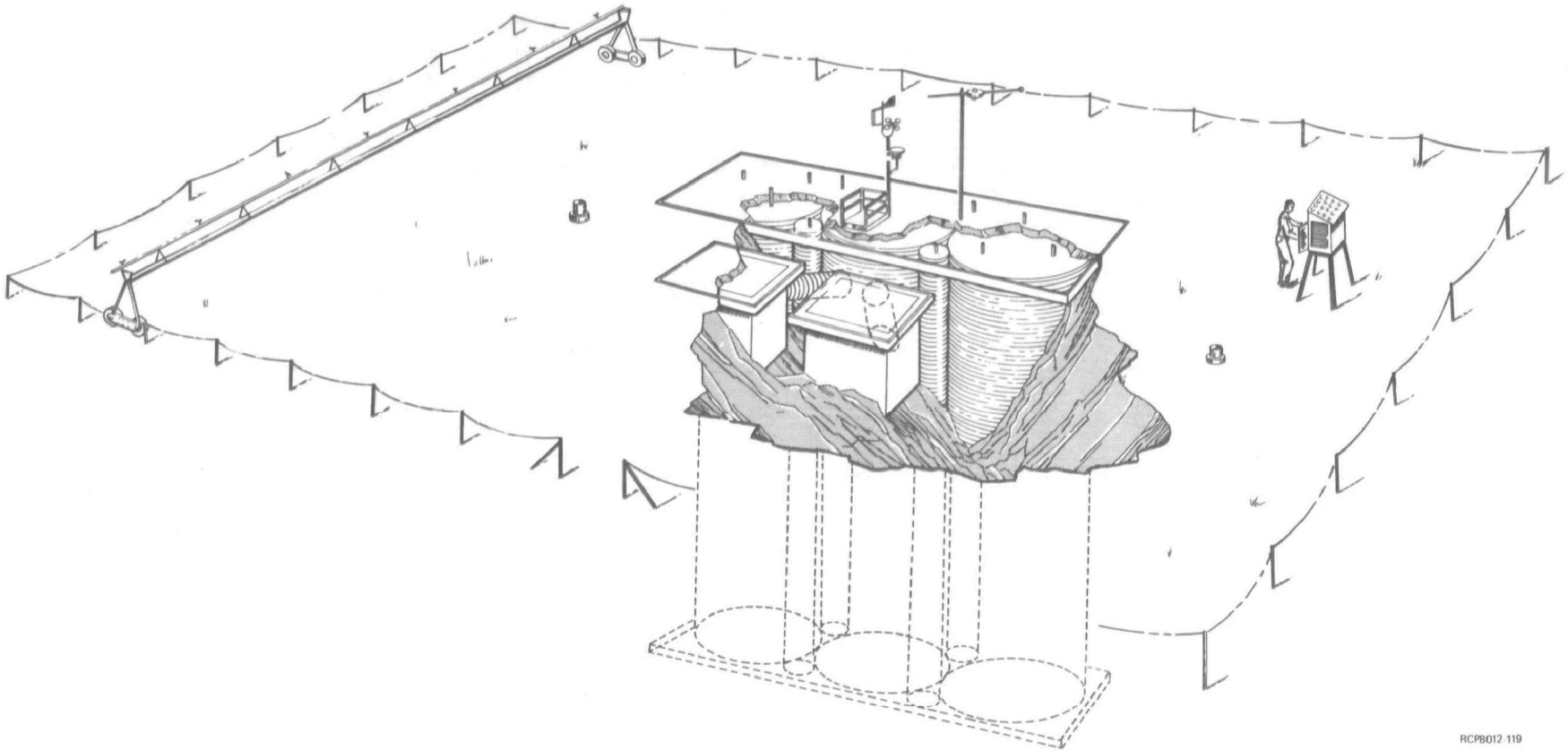

FIGURE 1. Oblique View Schematic of Shallow Facility Showing Caissons, Lysimeters, Micrometeorologic Instrument Sensors, etc.

layering effects. The remaining 6.0 m of the caisson were then backfilled with uniform sand. The four small caissons were excavated to a depth of 60.5 cm and a 1.0 cm layer of either cobalt-60 (^{60}Co), -ethylenediaminetetracetic acid (EDTA) or tritium (^{3}H) tagged backfill material was emplaced in alternating small caissons. The concentrations of respective radionuclides that were designed to function as liquid and vapor phase migration tracers were 6.4 $\mu Ci\ Kg^{-1}$ and 6.37 m $Ci\ Kg^{-1}$ at volumetric moisture contents equal to that of the larger caissons at the 60.0 cm depth. Excavated backfill material was then emplaced over the tagged layer.

During and subsequent to backfilling operations, active and passive monitoring access tubes, sensors and transducers were installed for: (1) neutron thermalization and sodium-iodide well logging, (2) geohydrological thermal and matric potential measurement, and (3) micrometerological thermal relative humidity, wind, precipitation, solar radiation, evaporation, etc. Passive monitoring procedures were developed and active data collected for computer processing.

Moisture migration and radionuclide transport occurs as a function of moisture content induced by changes in precipitation. In order to evaluate this function one-half of the facility field, in bilateral symmetrical configuration, was irrigated at twice the ambient precipitation rate at nearly ambient frequency.

MODIFIED UNSAT MODEL APPLICATION

Soon after construction of the Shallow Facility, modeling activities were completed to produce an initial prediction of water migration. A modified one-dimensional, isothermal, partially saturated, finite difference model was used[4,5]. Equations for total water flux were developed to account for thermal and matric potential gradients. Using a $-1.0\ cm\ cm^{-1}$ water potential gradient and equations for thermally induced water flux, a nonisothermal water flux in response to thermal gradients was calculated for various water contents in geologic media.

This suggested that simulation of isothermal conditions could adequately describe the flux of liquid water within the geologic media.

The following model simulating conditions in the caisson facility were used: (1) an 8.0 m profile of uniform sand with a coarse quartz sand layer, (2) a static water table at 8.0 m depth, (3) measured retentivity and saturated hydraulic conductivity values for the uniform and coarse quartz sand, (4) partially saturated hydraulic conductivity values as determined by the Millington and Quirk method[6], (5) the vapor flux from the surface was taken as 0.001 cm day^{-1}, (6) measured atmospheric temperature, wind, solar radiation, cloud cover, and precipitation, calculated potential and actual evaporation and (7) standard initial conditions of depth, suction head, volumetric water content, initial storage, final storage, infiltration, evaporation, and drainage. A model sensitivity analysis was also conducted to evaluate such factors as hydraulic conductivity, total precipitation, precipitation distribution, and layering.

DEEP CAISSON/DEEP WELL FACILITY

In 1971 a Deep Caisson/Deep Well Facility was designed to evaluate the migration of naturally occurring moisture in the partially saturated zone[7-10]. This Deep Caisson Facility has served as a one-dimensional structure amenable to partially saturated zone model simulation and verification. The Caisson Facility, Figure 2, shows geohydrological monitoring instrumentation. Near the Deep Caisson Facility is a deep instrumented well designed to monitor matric potential and temperature in geologic media between the surface and the water table. This instrumented well is also illustrated in Figure 2.

The Deep Caisson Facility consists of two thermally insulated caissons 3.0 m in diameter by 17.0 m in length buried below grade. Centrally located between these caissons is an instrument access caisson. Neutron thermalization access tubes and matric potential sensors were installed vertically through the two outer caissons. One caisson was sealed at its lowest extremity to form a liquid barrier, while the other remained open

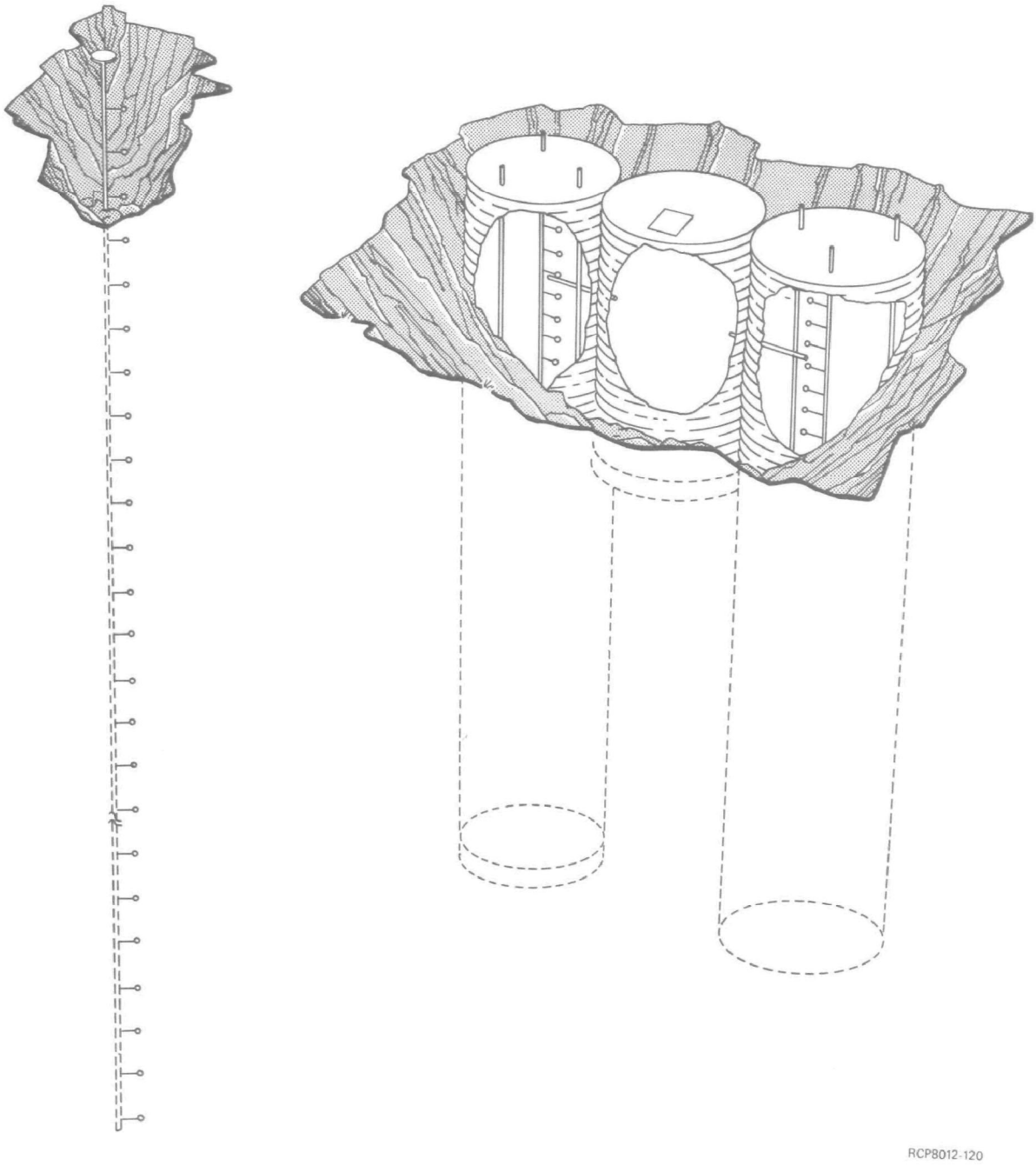

FIGURE 2. Oblique View Schematic of Deep Caisson/Deep Well Facility Showing Caissons and Geohydrological Instrument Sensors, etc.

so that direct communication between the ambient geohydrologic system would result. Uniform sand excavated during caisson construction and emplacement was backfilled into the two caissons.

A deep instrumented well was constructed to a depth of 97.0 m. Matric potential and thermal sensors were affixed to a cable and lowered into the well. The well was then backfilled with geologic media removed during construction.

MPHASE MODEL APPLICATION

In 1975 a computer code, MPHASE, was developed to simulate water migration through the Deep Caisson Facility. A one-dimensional, steady state, nonisothermal, liquid and vapor phase, partially saturated, finite element model formulation was used.[11] Equations were developed and modified for determination of saturation, total water flux and liquid and vapor phase fluxes. These equations accounted for thermal and diphasic water potential gradients. Dimensionless equations were formulated for: (1) water balance, (2) dry air balance, (3) energy balance, (4) liquid mass flux, (5) wet air mass flux and (6) dry air mass flux. Depth and time were also made dimensionless. A variable pressure, nonisothermal gradient for liquid and vapor phase flux was determined for all depths from the ground surface to the water table.

The MPHASE model used the following conditions: (1) 97^{o} m deep profile of homogeneous geologic media (2) static water table, (3) measured liquid and vapor hydraulic conductivities, (4) measured temperature, (5) measured capillary pressure and (6) fixed and/or time varying boundary conditions.

RESULTS AND DISCUSSION

MODIFIED UNSAT MODEL SIMULATION RESULTS

Sensitivity analyses of geologic media sand dependence on hydraulic conductivity to moisture migration at the shallow facility were performed

using ambient, 0.1 and 0.01 factors. Simulations demonstrated that: (1) water penetration into the geologic media was reduced by reducing the hydraulic conductivity by 0.1 or 0.01, (2) water storage and seepage below 2.0 m was not significantly affected, (3) a reduction in hydraulic conductivity reduced the water flow into the Shallow Facility so that it tended to remain closer to the ground surface and (4) a reduction in hydraulic conductivity resulted in reduced evaporation. Table 1 shows the results of varying hydraulic conductivity.

TABLE 1. Simulation Results of Varying Hydraulic Conductivity Values.[a,b]

Variable	Infiltration (cm)	Evaporation (cm)	Drainage (cm)	Storage (cm)
Ambient	24.1	26.3	-0.4	42.6
Ambient/10	24.5	23.3	-0.2	45.7
Ambient/100	24.5	22.7	-0.1	46.2

[a]Modified after Gee and Simmons, 1979

[b]Initial storage - 44.6 cm

Model simulations indicate that by varying the hydraulic conductivity there can be a pronounced effect on water content and flux near the ground surface, indicating these effects are reduced with depth. In addition, modification of hydraulic conductivity can, over time, influence the migration of water and nonsorbed radionuclides within geohydrologic systems.

The effects of annual precipitation in the form of rainfall were also evaluated by sensitivity simulations. The model, as anticipated, predicted that an increase in precipitation would increase drainage to the water table. The model results indicated: (1) changes of precipitation from one year to the next are reflected in the migration of moisture through and from the geologic media, (2) a significant decrease in annual precipitation below mean annual precipitation will propably result in negative

drainage of moisture to the water table whereas an increase will result in positive drainage, (3) moisture stored in the profile will not be drastically affected. The effect of total precipitation over six years using a one standard precipitation year value are shown in Table 2.

TABLE 2. Simulation of Total Precipitation Effects on Six Consecutive Years Based on Multiples of One Standard Precipitation Year.[a,b,c]

Year	Infiltration (cm)	Evaporation (cm)	Drainage (cm)	Storage (cm)
1	49.1 (2.0 x)	34.9	7.5	51.0
2	36.8 (1.5 x)	31.5	6.8	49.3
3	8.1 (0.33 x)	13.1	0.6	43.9
4	24.5 (1.0 x)	23.2	-0.3	45.5
5	36.8 (1.5 x)	30.9	1.9	49.3
6	18.5 (0.75 x)	21.1	1.0	45.6

[a]Modified after Gee and Simmons, 1979

[b]Initial storage - 44.6 cm

[c]Potential evaporation - 131.0 cm

Results of this simulation demonstrate that moisture migration is significantly affected by changes in total annual precipitation. Furthermore, annual precipitation history additionally affects moisture migration.

The sensitivity of the temporal distribution of precipitation on an annual basis was simulated in addition to the total annual precipitation. Two years with different temporal precipitation were selected, i.e., one year with precipitation occurring predominantly in the fall, year a, and the other with predominantly spring and winter precipitation, year b, as in Table 3. Model simulation results have indicated that by alternating years a and b variable increases or decreases of moisture evaporation, drainage and storage result depending on the alternation sequence. After using developed standard initial conditions and sequentially repeating

year a, moisture, evaporation, drainage and storage all increase. Model simulation results for alternative and repetitive years are shown in Table 3 and 4 respectively.

TABLE 3. Simulation of a Three-Year Precipitation Sequence.[a,b,c]

Year	Infiltration (cm)	Evaporation (cm)	Drainage (cm)	Storage (cm)
a	23.5	20.1	-0.1	48.0
b	24.6	25.0	0.7	46.7
c	24.0	24.6	0.2	46.4

[a]Modified after Gee and Simmons

[b]Initial storage - 44.6 cm

[c]Potential evaporation - 147.7 cm, year a; 131.2 cm, year b

TABLE 4. Simulation of a Three-Year Repetitive Precipitation.[a,b,c]

Year	Infiltration (cm)	Evaporation (cm)	Drainage (cm)	Storage (cm)
a	23.5	20.1	-0.1	48.0
a	23.5	22.0	1.2	48.2
a	23.5	22.1	1.3	48.2

[a]Modified after Gee and Simmons

[b]Initial storage - 44.6 cm

[c]Potential evaporation - 147.7 cm, year a; 131.2 cm, year b

The simulation indicates that the temporal distribution of precipitation significantly affects the hydrogeologic system. Furthermore, it illustrates the complexity of predictive modeling of systems with variable upper boundary layer conditions.

Sensitivity simulations were also completed to evaluate the effect of layering, relative to partially saturated moisture migration. Heterogeneity of geologic media in texturally alternating layers was found to

have a pronounced effect on moisture flux and drainage. Layering reduces the flux of liquid phase moisture across lateral layer boundaries during drainage, until the water saturation in the upper layer reaches some critical valve wherein the water will freely drain into the next lower vertical layer.

Model results indicate: (1) the interface between course and fine textured geologic media at a depth of 6.0 m significantly perturbates the moisture content profile, (2) drainage is reduced where a coarse layer exists in the profile while drainage is increased when this layer is omitted from the profile (3) storage of moisture in the profile is increased where the coarse layer is present; conversely, storage is reduced with omission of the coarse layer.

Simulation results of layering cases are shown in Table 5 for a non-homogeneous coarse geologic media layer between 6.0 m and 6.5 m in depth, (a) and a homogeneous profile (b).

TABLE 5. Simulations of Layering Effects.[a,b,c,d]

Water Table	Infiltration (cm)	Evaporation (cm)	Drainage (cm)	Storage (cm)	
				Initial	Final
(a)	23.5	20.1	-0.01	44.6	48.0
(b)	23.5	20.4	0.3	50.0	52.7

[a]Modified after Gee and Simmons, 1979

[b]Potential evaporation - 147.7 cm

[c]Coarse sand layer 600-650 cm

[d]Sand layer

Results of this sensitivity simulation demonstrate some of the effects of layering on the flux of moisture through, and the retention of moisture within, geologic media. These results may also provide insight into the utility of design of engineered barriers relative to the disposal of nuclear materials.

The UNSAT model simulations, using the configuration and data from the Shallow Facility, were used to provide an initial understanding and prediction of moisture migration and nonsorbed radionuclide transport in partially saturated geologic media.

Field data collected at the Shallow Facility over the past two years have shown: (1) the gravity potential dominates the flux of moisture through geologic media under both ambient and accelerated precipitation conditions, (2) low distribution coefficient ^{60}Co-EDTA has not been transported under ambient or accelerated precipitation conditions as calculated, (3) ^{3}H has been transported both in the vapor and liquid phase within the partially saturated profile of the facility, (4) ^{3}H has been transported in the liquid phase (data that suggests ^{3}H has also been transported in the vapor phase) within the partially saturated profile of the facility, (5) moisture in the liquid phase has accumulated in the bottom of the caissons receiving ambient plus two times ambient precipitation, where no accumulation of moisture has been found in the ambient precipitation caissons.

These simulation results are not intended to be conclusive. The results were derived using actual and assumed data from the Shallow Facility and adjacent experimental sites soon after construction. The purpose of modeling this system was to provide an approximation of moisture migration and nonsorbed radionuclide transport at the Shallow Facility. These data could then be used to develop monitoring systems. The model results also increased our understanding of the mechanism of flow in geologic media under various conditions.

MPHASE MODEL SIMULATION RESULTS

Steady state and transient simulations of liquid and vapor phase moisture flux were performed for both the open and closed bottom caissons of the Deep Caisson Facility. Model solutions for the open bottom caisson during steady state conditions yielded applicable results while solutions for the closed bottom caisson were found to require further model

development. Steady state simulation results indicated: (1) near the ground surface moisture migration is predominantly in the vapor phase, (2) liquid phase moisture flux in the caisson is upward but is extremely small, (3) vapor phase migration throughout the profile is upward at a nearly constant rate, liquid phase flux below the caisson is downward at a rate lower than that of the vapor phase, and (5) the total flux is upward.

Table 6 shows dimensionless values for liquid and vapor fluxes versus saturation at various depths. The caissons extend to a dimensionless depth of 0.16.

TABLE 6. Vapor and Liquid Phase Flux vs. Saturation at Various Depths in Deep Open Bottom Caisson (Dimensionless Values).[a,b]

Depth	Saturation	Liquid Flux	Vapor Flux	Total Flux
0.0000	0.0600	-1.843 (-12)	-1.307 (-7)	-1.307 (-7)
0.1154	0.0600	-8.670 (-12)	-1.307 (-7)	-1.307 (-7)
0.3846	0.0600	2.019 (-10)	-1.309 (-7)	-1.307 (-7)
0.5000	0.0600	1.186 (-9)	-1.319 (-7)	-1.307 (-7)
0.6154	0.0600	2.997 (-9)	-1.314 (-7)	-1.284 (-7)
0.8846	0.0611	1.091 (-8)	-1.393 (-7)	-1.282 (-7)
1.0000	1.0000	-1.307 (-7)	0.000	-1.307 (-7)

[a]Modified after Finlayson, 1975

[b]Dimensionless flux x 5.5×10^{-4} = g sec^{-1}

The total flux was found to be quite dependent on the pressure gradient that determines the direction of liquid mass flux. This relates whether the pressure gradient is greater or less than the gravitational force acting on the liquid.

Continued monitoring of variables controlling moisture migration at the Deep Caisson Facility could yield results amenable to model calibration and verification.

CONCLUSIONS

Field monitoring and model simulations of moisture migration and radionuclide transport and controlling factors are exceedingly complex. This is indicated by the variability of model simulations and model sensitivity simulations reported herein. Presently only limited simulation and prediction estimates of migration and transport can be made.

Further field, laboratory and model development efforts will enhance the capability to simulate, predict, error bound and verify moisture migration and radionuclide transport under field conditions at the Hanford Site.

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RADIONUCLIDE TRANSPORT UNDER CHANGING SOIL SALINITY CONDITIONS*

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SUMMARY

This paper presents experimental measurements and computer simulations of strontium-85 movement through laboratory soil columns. There are two primary objectives of the work. The first is to examine the enhanced mobility of strontium-85 when the soil salinity is raised. The second is to compare the ability of two solute transport models to describe this phenomena. The experiment consisted of injecting a pulse of what will be termed a "low salt" solution spiked with strontium-85 into a soil column. The column was then leached with over eighteen pore volumes of the low salt solution resulting in no leaching of the strontium-85 from the column. Subsequently, the column was leached with a "high salt" solution, causing the rapid release of the strontium-85 within five to six pore volumes.

These data were analyzed using models based on two sets of equations. The first used the traditional convective dispersive equation. This equation contains the three parameters; water velocity V, dispersion coefficient D, and the distribution coefficient Kd. The first two may be combined to form the dimensionless Peclet number (P)' and the Kd is often expressed as a dimensionless retardation factor (R). This equation in dimensionless form is a two parameter solute transport equation. The second model uses the mobile-immobile water equation described by Van Genuchten and Wierenga (1976a). This model uses a set of two equations which contain six parameters which may be combined into four dimensionless parameters.

These models involve a large number of parameters that must be evaluated. The techniques used in this work used the curve fitting routine described by van Genuchten (1980), as well as some batch Kd measurements described by Gee and Campbell (1980). The curve fitting was done on breakthrough curves obtained from separate column leachings with strontium and tritium using the high salt solution. The parameter

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*Prepared for the U.S. Department of Energy under contract DE-AC06-76RLO-1830.

estimates were then used in the low salt-high salt experiment described above. This follows the reasoning outlined by van Genuchten and Wierenga (1977a, 1977b).

The results demonstrate that strontium-85 is subject to greater mobility when the soil salinity is increased. This confirms the necessity of evaluating the soil salinity very carefully in modeling efforts. The results also indicate that batch Kd values, combined with column Kd values and parameters obtained by curve fitting procedures do a fairly good job in describing the "snowplow effect." The comparison of the two models reveal insignificant differences when describing the movement of tritium and strontium-85 under high salinity conditions. There was a significant improvement, however, when the mobile-immobile water equations were used to describe the combined low salt-high salt experiment.

INTRODUCTION

The characterization of sorption reactions that remove radionuclides from solution in soils and sediments is a very active area of research. Among the diverse processes being studied are oxide and carbonate precipitation, precipitation of hydroxide compounds, coprecipitation with amorphous hydrous oxides, lattice replacement, and ion exchange. In recent years the relative emphasis placed on ion exchange has decreased, however, it still is an important process for certain radionuclides. A fundamental property of ion exchange reactions is that they are dependent on the solution concentration of the exchanging ion as well as the ionic strength and composition of the bulk solution. The general trend of strontium-85 observed by Gee and Campbell (1980) was for the sorption (i.e., Kd value) to increase with increasing ionic strength of the bulk solution. This would indicate that ion exchange plays some role in the sorption of strontium-85.

The implication for shallow land burial sites is that errors can be made in predicting the movement of some radionuclides through sandy soils when only average salt concentrations are used in predictive equations rather than actual time dependent salt concentration. Burial ground soils with relatively high concentrations of salt may, under increased rainfall, flush sorbed radionuclides from the soil exchange sites creating a much higher effluent concentration than predicted. This flushing action by a high salt concentration influent solution has been called the "snowplow effect" (Starr and Parlange 1979). Included in this report is verification of the "snowplow effect" for strontium-85. Conventional solute transport equations and those that include the mobile and immobile water concept (Van Genuchten and Wierenga 1976b), are used to analyze the data.

Materials and Soil

The soil used in this experiment was a coarse sand found at the Hanford site. This soil is classified as a typic torripsament. The clay content is <4%, the cation exchange capacity is approximately 5 meq/100 g and the soil pH is 8.2.

The solutions used in the tests were two mixed salt solutions designated as low (L) and high (H) salt. The two solutions had the following compositions:

Low salt (L) — 0.15M $NaNO_3$, 0.01M KNO_3, 0.002M $Ca(NO_3)_2$

High salt (H) — 0.15M $NaNO_3$, 0.15M KNO_3, 0.01M $Ca(NO_3)_2$

The experimental equipment used to demonstrate the snow plow effect was designed after that used by Van Genuchten and Wierenga (1977a,b). This is the same design described in Gee and Campbell (1980). Influent solutions were applied at the upper end of soil columns packed in plexiglass cylinders of 5.4 cm inside diameter. Columns 27.5 cm long of Rupert sand were packed to a dry bulk density of 1.73 g/cm^3. At the lower end of the vertically positioned column, a porous plate for controlling vacuum and supporting the soil was attached. The column was connected to a vacuum chamber enclosing an automatic fraction collector. Figure 1 shows the apparatus used for measuring radionuclide transport in unsaturated soil.

The low salt solution containing a 50 nci/mℓ spike of strontium-85 was pumped through the column. After 4.3 pore volumes were injected, the strontium-85 was removed from the influent solution. The column was maintained at a moisture content of 0.17 cm^3/cm^3, and the flow rate was 6.8 cm/day. After 18.25 pore volumes of effluent were collected, the relative concentration of strontium-85 (C/C_0) was <0.01. The high salt solution containing no strontium-85 was then added to the column at a flow rate of 7.0 cm/day. The effluent was collected and the breakthrough curve determined.

The results of the low-salt, high-salt experiment are shown in Figure 4. The data show quite clearly the rapid release of strontium-85 after the addition of the high salt solution at 18.25 pore volumes. The rapid rise in effluent concentration and the C/C_0 value >1 are manifestations of this showplow effect. The two curves shown represent the curves predicted by the two and four parameter models. The parameters used in the simulations are discussed in the next section. Figure 4 shows a distinct improvement in describing the snowplow effect by using the four parameter model. Neither model predicts the fast rise of the curve or the $C/C_0 > 1$. The four parameter model does however do a good job of describing the tailing.

COMPUTER SIMULATION

The computer models used for this simulation are described in detail by Van Genuchten and Wierenga (1974, 1976b) and Van Genuchten (1980). They were written using the IBM system 360 Continuous Systems Modeling Program (S/360 CSMP), simulation language. The first model used the convective dispersive equation:

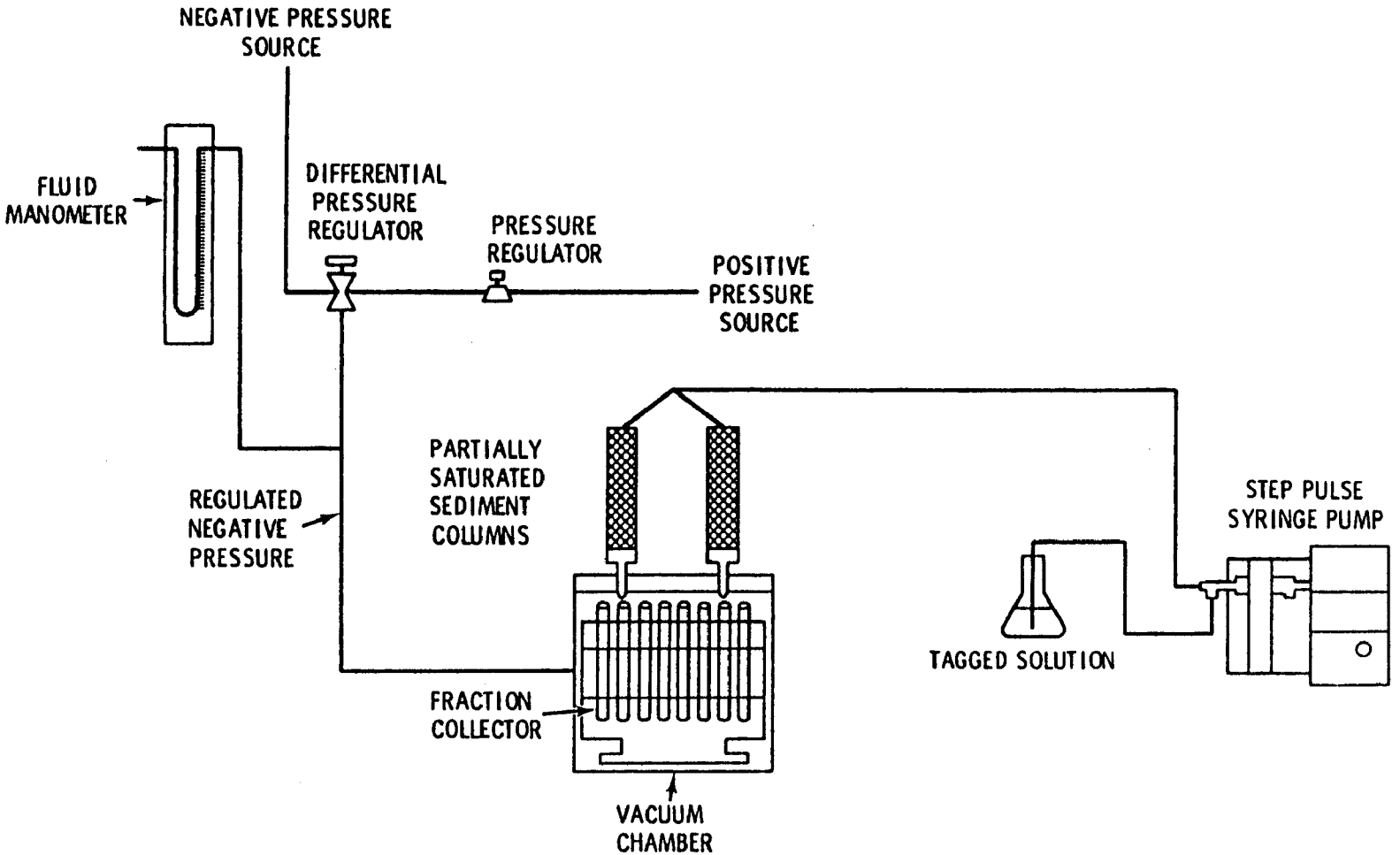

Fig. 1. Apparatus for measuring radionuclide movement in unsaturated soil columns.

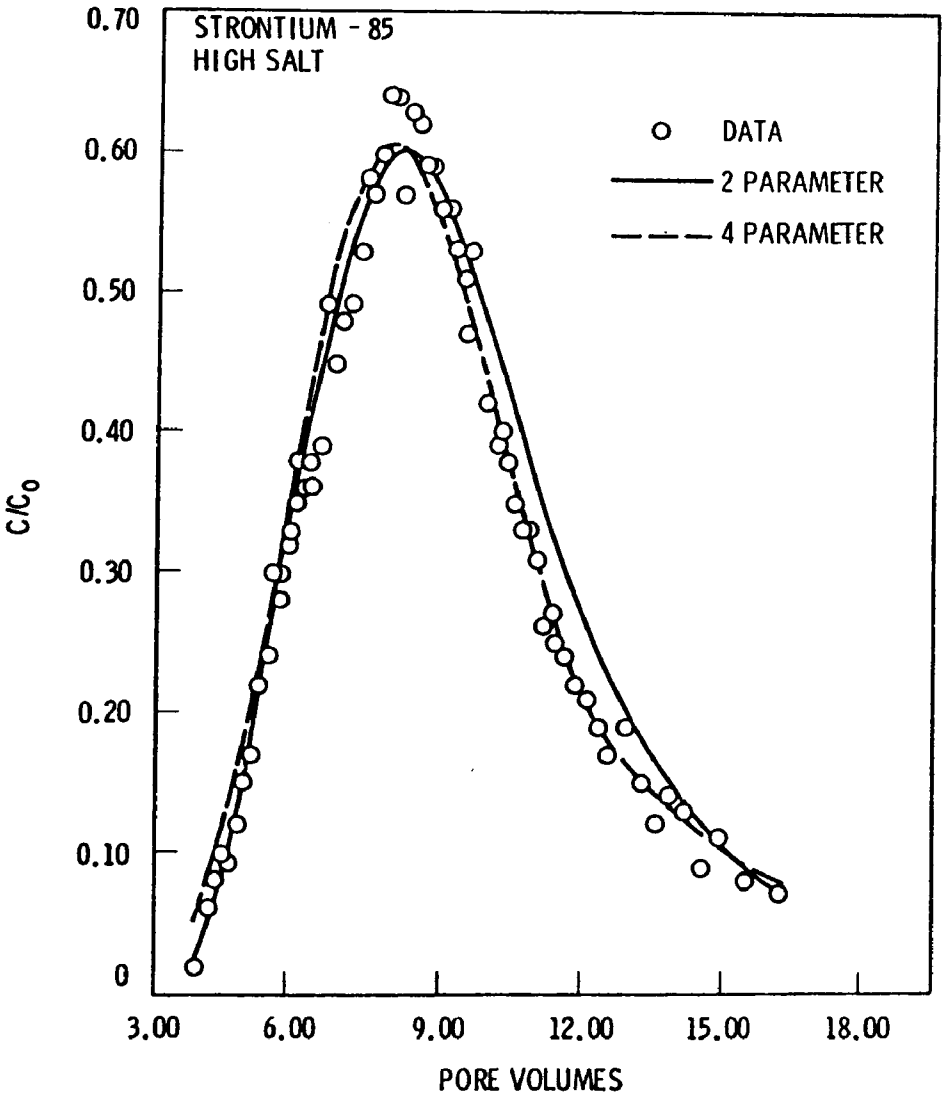

Fig. 2. High salt strontium breakthrough curve.

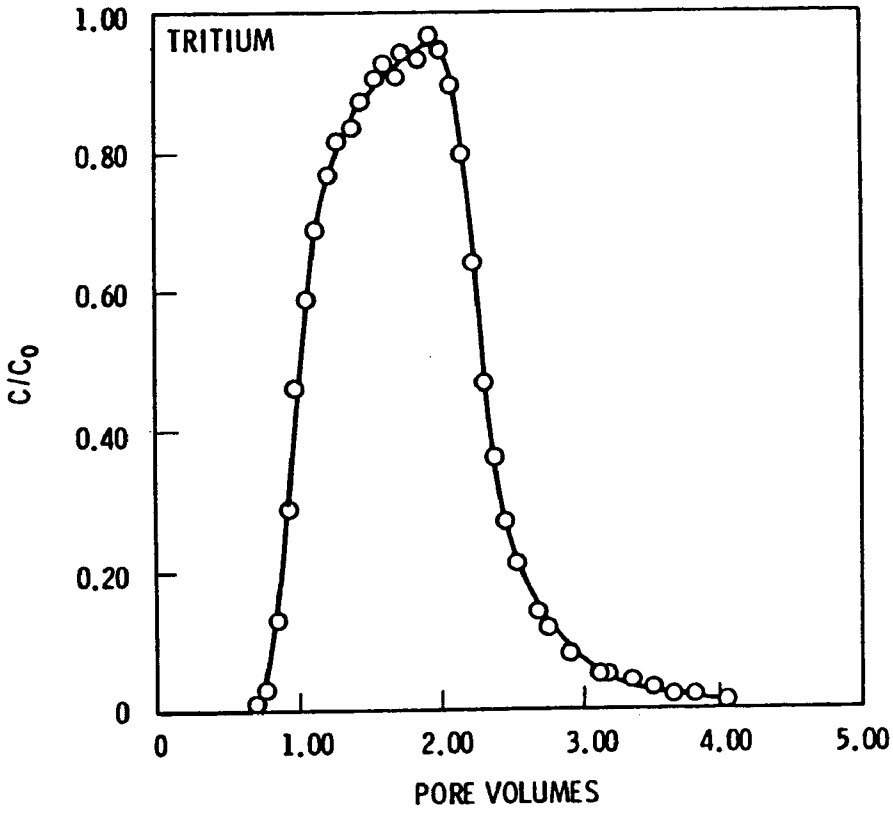

Fig. 3. High salt tritium breakthrough curve.

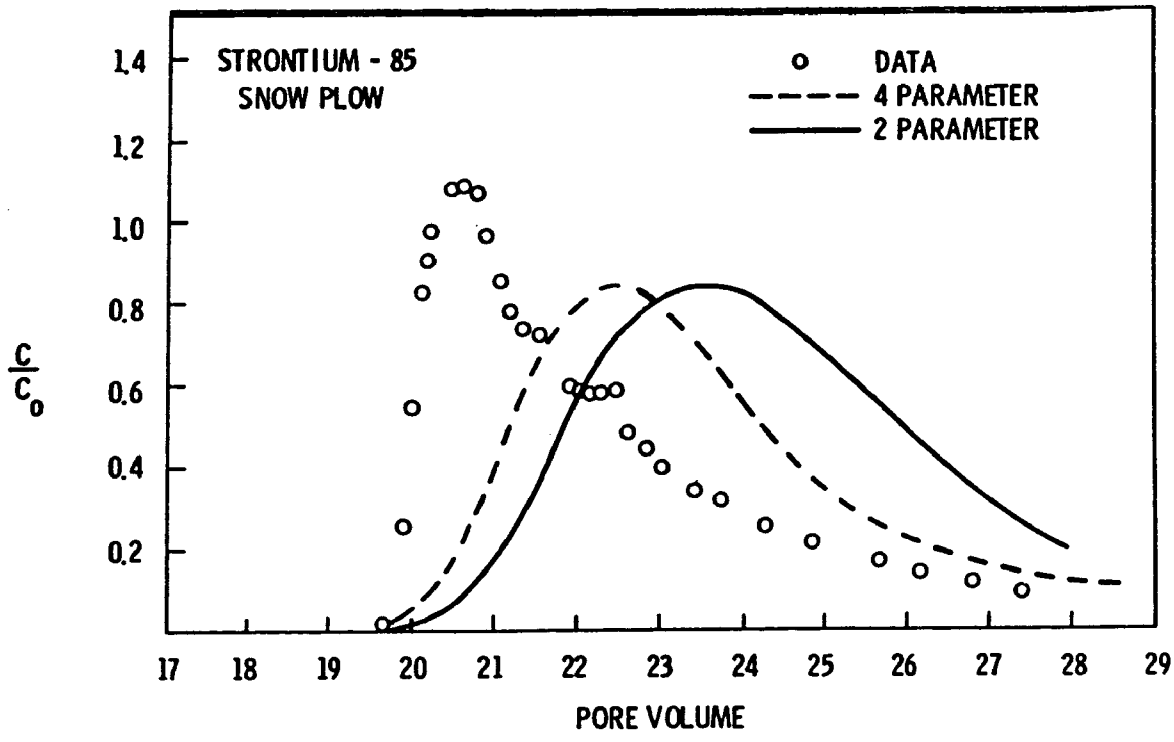

Fig. 4. Comparison of two and four parameter fit for snowplow effect.

$$\left(1 + \frac{pKd}{\theta}\right) \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - \frac{v \partial C}{\partial x} \tag{1}$$

where

C = concentration of solute

t = time

x = vertical distance from surface

D = dispersion coefficient

v = pore water velocity

P = bulk density

θ = volumetric water content

Kd = radionuclide distribution coefficient

in dimensionless form this becomes

$$R \frac{\partial C}{\partial T} = \frac{1}{P} \frac{\partial^2 C}{\partial X^2} - \frac{\partial C}{\partial X} \tag{2}$$

where

$$R = 1 + \frac{pKd}{\theta} \tag{3}$$

$$P = 1 + \frac{vL}{D} \quad (L = \text{Length of Column}) \tag{4}$$

$$T = \frac{vt}{L} \tag{5}$$

$$X = \frac{x}{L} \tag{6}$$

The second model used the mobile-immobile water equations of Van Genuchten and Wierenga (1976b):

$$(\theta_m + fpKd) \frac{\partial Cm}{\partial t} + (1-\theta)_m + (1-f)pKd \frac{\partial C_{im}}{\partial t} = \theta_m D \frac{\partial^2 C_m}{\partial X^2} - V_m \theta_m \frac{\partial C_m}{\partial X} \tag{7}$$

and

$$\theta_{im} + (1-f)pKd \frac{\partial C_{im}}{\partial t} = \alpha (C_m - C_{im}) \tag{8}$$

where

θ_m = mobile water fraction

f = fraction of exchange sites in contact with mobile water

C_m, C_{im} = solute concentration in mobile and immobile water phase

V_m = mobile water velocity

α = mass transfer coefficient

in dimensionless form these equations become:

$$\beta R \frac{\partial c_m}{\partial T} + (1-\beta)\, R \frac{\partial c_{im}}{\partial T} = \frac{1}{P} \frac{\partial^2 c_m}{\partial X^2} - \frac{\partial c_{im}}{\partial X} \tag{9}$$

$$(1-\beta)\, R \frac{\partial c_{im}}{\partial T} = \bar{\alpha}\, (c_m - c_{im}) \tag{10}$$

$$\bar{\alpha} = \frac{\alpha L}{V_m \theta_m} \tag{11}$$

$$\phi = \frac{\theta_m}{\theta} \tag{12}$$

$$\beta = \frac{\phi + (R-1)f}{R} \tag{13}$$

$$c_{im} = \frac{C_{im}}{C_o} \tag{14}$$

$$c_m = \frac{C_m}{C_o} \tag{15}$$

C_o = radionuclide concentration of influent solution

The parameters used for the convective dispersive equation were obtained by curve fitting an analytical solution (Van Genuchten 1980), of Equation 2 to the data shown in Figure 3. This produced estimates of 19 for P and 7.2 for R. The CSMP model used Equation 1 so Equations 3 and 4 were used to calculate R. The CSMP model used Equation 1 so Equations 3 and 4 were used to calculate Kd and D. The pore water velocity was measured during the experiment to be 6.7 cm/day, and the column length was 27.5 cm. These calculations are summarized in Table 1. There was no breakthrough curve available for the low salt solution so the batch Kd value of 6 was used and the high salt D value was used. The CSMP model was used to track both the salt concentration

of the bulk solution and also the radionuclide solution. As the soil salinity increased from low to high as the high salt solution moved through the column, the Kd value was assumed to vary linearly from 6 to 0.6.

The parameter values for the mobile-immobile water equations were obtained in a similar way. An analytical solution (Van Genuchten and Wierenga 1976b), of Equations 9 and 10 was curve fit to the data in Figures 2 and 3. The CSMP model used Equations 7 and 8 so a conversion using equations 3, 4, 11, and 13 was done. The only conversion which is not straightforward is the use of Equation 13. The value of B and R from the tritium experiment was used first. Assuming $0 \leq f \leq 1$, we calculate a range of $\emptyset$ of 0.84 to 0.95. Assuming $\emptyset$ is the same for tritium and strontium, we then use β and R from the high salt strontium data. Assuming $0.84 \leq \emptyset \leq 0.95$, we obtain a range for f of 0.69 to 0.7. The simulation of the snowplow experiment used $\emptyset = 0.9$ and $f = 0.7$.

CONCLUSIONS

Radionuclide transport under changing soil salinity conditions was investigated by using two solute transport equations to describe the transport of strontium-85 through laboratory columns. The two parameter convective dispersive equation was compared to the four parameter mobile-immobile water equations of Van Genuchten and Wierenga (1976a).

Both models were relatively successful in describing the rapid flush of strontium-85 from a column with a high salt solution, a phenomena called the snow plow effect. This effect was simulated by using a Continuous System Modeling Program (CSMP) simulation model to solve the two equations. The four parameter mobile-immobile water model predicted the release of the strontium more accurately, but neither model predicted the peak effluent concentration well. Both models confirm enhanced mobility of strontium-85 with increased salt concentration of leaching waters.

Table 1. Parameter Estimates for Computer Simulations

	P	R	β	$\bar{\alpha}$	D	α	Kd	θm	f
Tritium	106	1.1	0.9	0.4	-	-	-	0.9	0.5
Strontium-85									
2 parameter	19	7.2	-	-	58	-	0.6	-	-
4 parameter	29	8.4	0.7	0.5	41	0.12	0.74	0.9	0.7

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ON THE COMPUTATION OF THE VELOCITY FIELD AND MASS BALANCE IN THE FINITE-ELEMENT MODELING OF GROUNDWATER FLOW

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ABSTRACT

Darcian velocity has been conventionally calculated in the finite-element modeling of groundwater flow by taking the derivatives of the computed pressure field. This results in discontinuities in the velocity field at nodal points and element boundaries. Discontinuities become enormous when the computed pressure field is far from a linear distribution. It is proposed in this paper that the finite element procedure that is used to simulate the pressure field or the moisture content field also be applied to Darcy's law with the derivatives of the computed pressure field as the load function. The problem of discontinuity is then eliminated, and the error of mass balance over the region of interest is much reduced. The reduction is from 23.8 to 2.2% by one numerical scheme and from 29.7 to -3.6% by another for a transient problem.

INTRODUCTION

To study the transport of dissolved constituents in a subsurface flow system, the velocity field therein must be determined first. Several finite-element Galerkin models have been developed to obtain the flow field [1-8]. The continuity equation of water-mass governing the distribution of pressure head was solved by the Galerkin finite-element method, subject to appropriate boundary and initial conditions. The flow field was computed with Darcy's law by taking the derivatives of the calculated pressure field [3-6]. Inherent in that approach, however, was the resulting discontinuity in the velocity at nodal points and element boundaries, which unfortunately lead to a violation of the conservation of mass in a local sense. Results from two hypothetical sample problems showed that the discontinuity in the velocity field obtained by the conventional approach ranges from very small to several hundred percent depending on the location in the region. Furthermore, the overall mass balance is not preserved. When spatial distribution of the velocity is significant, inputting this discontinuous flow field to the contaminant transport computation could conceivably produce large error.

It is proposed to solve Darcy's law for the velocity field at nodal points by the same finite-element method used for the pressure field rather than simply to take the derivatives of the approximate pressure field. This approach is consistent with the spirit of finite-element modeling of groundwater flow. It also yields a continuous velocity field over the region of interest including nodal points and element boundaries. Accordingly, this paper describes the use of the finite-element method, as applied to Darcy's law, to remove the discontinuity described above. The two hypothetical problems are reexamined in the light of the proposed approach, and the results are presented.

MATHEMATICAL STATEMENT

The governing equations to describe the water movement in variably saturated-unsaturated porous media have been derived in detail [4] in the following form:

$$F \frac{\partial h}{\partial t} - \partial_i [K_{ij} \partial_j H] - Q = 0 \tag{1}$$

and

$$V_i = -K_{ij} \partial_j H \quad , \tag{2}$$

where

$$F = \frac{\theta}{n} \alpha' + \beta' + \frac{d\theta}{dh} \tag{3}$$

and

$$H = h + z \quad , \tag{4}$$

in which h is the pressure head, θ is the moisture content, n is the effective porosity, α' and β' are the modified coefficients of compressibility of the medium frame and water, respectively, K_{ij} is the hydraulic conductivity tensor, V_i is the Darcian velocity vector, t is the time, Q is the artificial recharge or withdrawal, z is vertical coordinate, and H is the total head. In Eqs. (1) and (2),

∂_i denotes the partial differentiation with respect to the spatial coordinate, x_i; and $z = x_3$ is the vertical coordinate. In general, Eq. (1) is nonlinear because both the soil property, F (represented by Eq. (3)), and hydraulic conductivity tensor, K_{ij}, are nonlinear functions of the pressure head, h.

The initial condition of Eq. (1) may take the following form:

$$h = h_o(x_i) \qquad \text{in} \quad R \ , \tag{5}$$

where h_o is a prescribed function of the spatial coordinate, x_i, R is the region of interest enclosed by the boundary, $B(x_1, x_2, x_3) = 0$ as shown in Fig. 1. The function, h_o, may also be obtained by simulating the steady-state version of Eq. (1) with time-invariant boundary conditions. In the groundwater flow model, three types of boundary conditions are generally encountered. On the first type (Dirichlet) boundary, the pressure head is prescribed:

$$h = h_1(x_i,t) \qquad \text{on} \quad B_1 \ , \tag{6}$$

where B_1 is a portion of the boundary B and h_1 is a given input function of time and spatial coordinate on B_1. On the second type (Neumann) boundary, the flux is prescribed as:

$$- n_i \cdot K_{ij} \cdot \partial_j H = q_2 \qquad \text{on} \quad B_2 \ , \tag{7}$$

where n_i is the directional cosine of the outward unit vector normal to the B_2 portion of the boundary B. The third type is the variable boundary in the sense that either the Dirichlet or the Neumann conditions may prevail:

$$h = h_3(x_i,t) \qquad \text{on} \quad B_3 \tag{8a}$$

or

$$- n_i \cdot K_{ij} \cdot \partial_j H = q_3 \qquad \text{on} \quad B_3 \ , \tag{8b}$$

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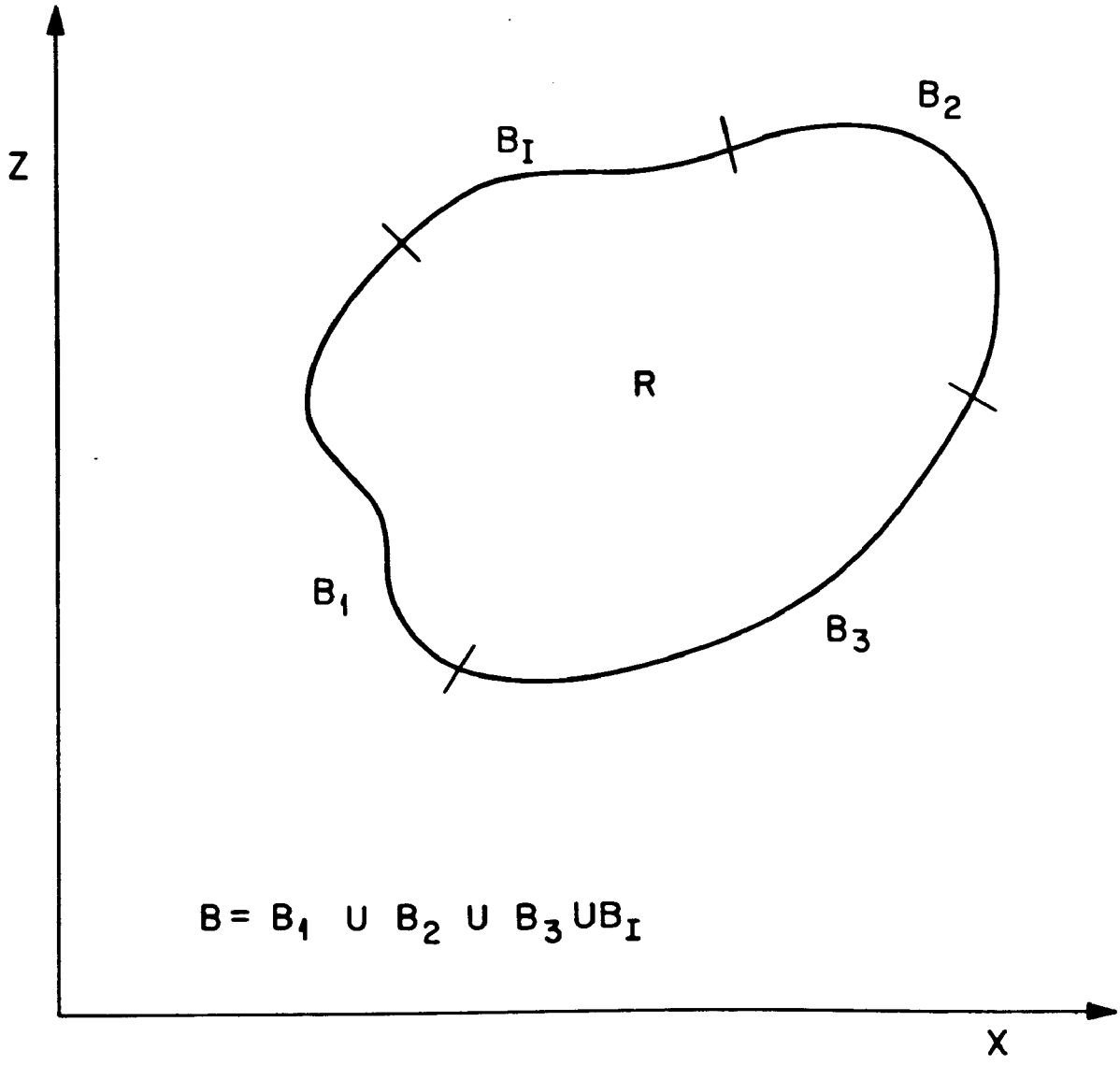

Fig. 1. Spatial boundaries, B_1, B_2, B_3, and B_I, of flow region R. (B.C. = Boundary Conditions).

where h_3 and q_3 are two known input functions of time and spatial coordinate x_i 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, $B(x_1, x_2, x_3) = 0$. Initially Eq. (8a) is applied to the boundary B_3 when the exact boundary conditions cannot in general be predicted a priori. Such a case would arise at the ground surface where either ponding (Dirichlet) or infiltration (Neumann) conditions could prevail [6]. This can only be determined in the cyclic process of solving Eqs. (1) and (2).

Applying the Galerkin finite-element procedure to Eq. (1), one obtains the following matrix equation:

$$[M_{ij}]\{\dot{h}_j\} + [S_{ij}]\{h_j\} + \{D_i\} + \{Q_i\} = 0 \quad , \tag{9}$$

where the temporal derivative of the head, h_j is given by

$$\dot{h}_j = \frac{dh_j}{dt} \quad . \tag{10}$$

The matrix equation coefficients are defined as:

$$M_{ij} = \int_R N_i F N_j \, dR \quad , \tag{11}$$

$$S_{ij} = \int_R \{(\partial_m N_i)\cdot K_{mn}\cdot(\partial_n N_j)\} dR \quad , \tag{12}$$

$$D_i = \int_R [K_{m3}\cdot(\partial_m N_i) - QN_i] \, dR, \quad \text{and} \tag{13}$$

$$Q_i = \int_{B_2} N_i q_2 \, dB + \int_{B_3} N_i q_3 \, dB \quad , \tag{14}$$

where N_i is the basis function at the nodal point i.

Eq. (9) can be solved by any of the six alternative numerical schemes listed in Table 1 [8]. They are dependent on the method of time marching and the treatment of the mass matrix, $[M_{ij}]$. For example, scheme 1 uses the central difference time marching with no mass lumping for the matrix, $[M_{ij}]$.

After the pressure field, h, is obtained, the Darcian velocity can be obtained by Darcy's law, Eq. (2). Conventionally, it is evaluated numerically by taking the derivative of the approximate pressure field, $h = h_k N_k$, as follows:

$$V_i = -K_{ij} [\partial_j (h_k N_k) + \delta_{j3}] \tag{15}$$

This approach naturally yields the discontinuity in the velocity, V_j, at nodal points and element boundaries. If continuity is to be achieved, the nodal gradient must also be treated as an unknown [6]. This in turn will increase, by a factor of 3 in the two-dimensional problems or 4 in the three-dimensional problems, the number of equations and the bandwidth of the system and thereby increase drastically the computing time and computer storage requirements. To circumvent this problem, it is proposed that the finite-element method be applied to Eq. (2) to yield:

$$[S'_{ij}]\{V_{nj}\} = \{D_{ni}\} \qquad n = 1, 2, \text{ or } 3 \quad , \tag{16}$$

where

$$S'_{ij} = \int_R N_i N_j \, dR \tag{17a}$$

and

$$D_{ni} = - \int_R N_i [K_{nm} \{\partial_m (N_j h_j) + \delta_{m3}\}] \, dR \tag{17b}$$

Eqs. (9) and (16) can be solved simultaneously by iteration. This will not complicate the problem, since Eq. (9) has to be solved iteratively because of its nonlinearity for each time step. It will not require any additional storage either. However, it will increase the CPU time by a factor of less than 3 or 4 for two- and three-dimensional problems respectively. If the storage for the matrix $[S_{ij}]$ is available, the CPU time will remain practically the same as the conventional approach, because $[S_{ij}]$ needs to be evaluated and triangularized only once.

The mass balance over the whole region of interest is obtained by integrating Eq. (1):

$$\int_R F \frac{\partial h}{\partial t} \, dR = \int_B F_n \, dB \quad , \tag{18}$$

where F_n is the normal flux through the global boundary $B(x,z) = 0$. In fact, F_n denotes:

$$F_n = n_i \, K_{ij} \, \partial_j H \quad . \tag{19}$$

Having obtained the pressure head field, h, one could integrate the rightand left-hand sides of Eq. (18) independently. If the solution for h is free of error, one would expect the equality of the two integrals. In this paper, the integral of the right-hand side is broken into five components:

$$F_D = \int_{B_1} F_n \, dB \quad , \tag{20}$$

$$F_N = \int_{B_2} F_n \, dB \quad , \tag{21}$$

$$F_S = \int_{B_{3S}} F_n \, dB \quad , \tag{22}$$

$$F_R = \int_{B_{3R}} F_n \, dB \quad , \text{ and} \tag{23}$$

$$F_I = \int_{B_I} F_n \, dB \quad , \tag{24}$$

where F_D, F_N, F_S, F_R, and F_I represent the fluxes through the Dirichlet boundary, B_1; the Neumann boundary, B_2; the seepage boundary, B_{3S}; the rainfall-infiltration boundary, B_{3R}; and the impervious Neumann boundary, B_I; respectively. On the other hand, the integral on the left-hand side of Eq. 18,

$$F_V = \int_R F \frac{\partial h}{\partial t} dR \quad , \tag{25}$$

represents the volumetric increasing rate of the moisture content in the region. For exact solution, the net flux across the whole boundary, defined by

$$F_{net} = F_D + F_N + F_S + F_R + F_I \tag{26}$$

should satisfy the following equation:

$$F_{net} = F_V \quad . \tag{27}$$

In addition, F_I should theoretically be equal to zero. However, in any practical numerical simulation, Eq. (27) will not be satisfied and F_I will be nonzero. Nevertheless, the mass balance computation should provide a means to check the numerical scheme and consistency in the computer code.

RESULTS

Two sample problems are used to compare the results from the models represented by Eqs. (15) and (16), respectively. The first example is a hypothetical seepage pond problem described earlier [9]. The second one is the Freeze's transient problem reported elsewhere [4,10]. In addition, results by all six alternative numerical schemes (Table 1) are compared in both examples.

Seepage Pond Problems

A seepage pond is assumed to be situated entirely in the unsaturated zone above a water table (Fig. 2a). This pond provides a source

Table 1. Listing of Alternative Numerical Schemes

Numerical schemes	Time-marching			Mass matrix	
	Central difference	Backward difference	Mid-difference	Without lumping	With lumping
1	X			X	
2		X		X	
3	X				X
4		X			X
5			X	X	
6			X		X

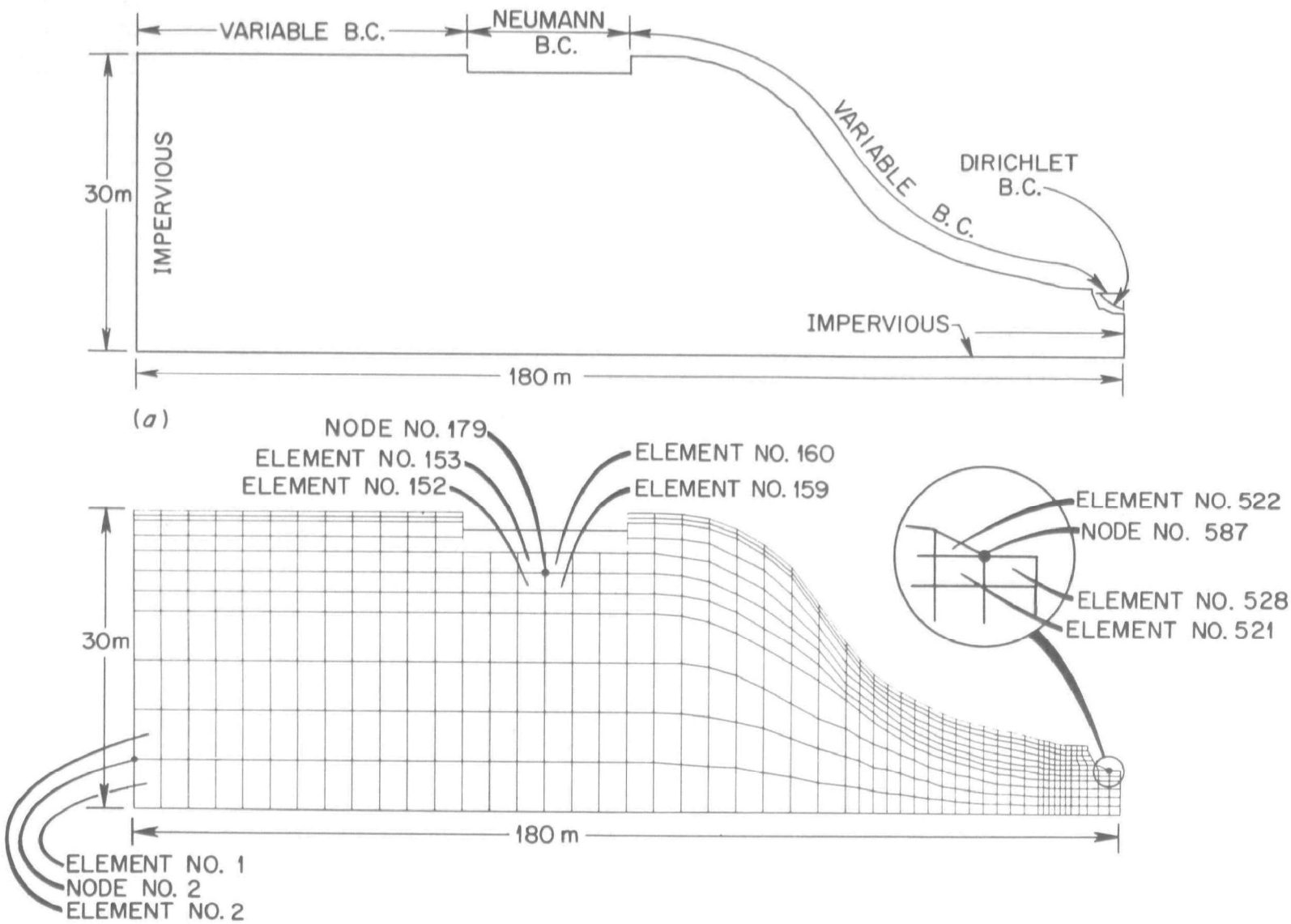

Fig. 2. Spatial discretization of the seepage pond problem.

of water which infiltrates into subsurface aquifers. After water reaches the water table, it flows toward a stream. Is is further assumed that the system is composed of highly permeable sand with soil properties shown in Fig. 3. For the finite-element computation, the entire region is discretized by 595 nodal points and 528 elements (Fig. 2b). Seven nodal points on the stream-soil interface are designated as Dirichlet nodes. Seven nodal points on the bottom of the seepage pond are considered as constant Neumann flux points and are assigned a constant infiltration rate of 4.0×10^{-4} cm/s. The top sides of all elements on the sloping surface, except the two elements immediately to the right of the seepage pond, are considered variable boundary surface, i.e., seepage-rainfall boundary. In other words, the nodal points on this surface are either Dirichlet or Neumann points with the infiltration rate equal to the excess rainfall rate.

The Darcian velocity field computed by model Eq. (15) shows the discontinuity at every nodal point as indicated by multivectors at any point in Fig. 4. The severity of this discontinuity depends on the location. This discontinuity is completely eliminated with model Eq. (16) as can be seen from Fig. 5, which shows the unique velocity vector at all nodal points. Table 2 shows the comparison of the computed Darcian velocity components simulated by model Eq. (15) and (16), respectively, for the three selective nodal points 2, 179 and 587 (Fig. 2). These three sample points are taken from computer output to illustrate the difference between the two models. It is seen that at nodal point no. 2, the vertical velocity component as computed from element no. 2 is about 2.58 times that computed from element no. 1. The values of the horizontal component, V_x, at nodal point no. 179 as computed from element nos. 159 and 160 are about 1.41 times those computed from element nos. 152 and 153; while the values of the vertical component, V_z, at the same point as computed from element nos. 153 and 160 are about 4.69 times those computed from element nos. 152 and 159. At nodal point no. 587, the vertical velocity component, V_z, as computed from element no. 522 is about 1.27 times that computed from element nos. 521 and 528. On the other hand, results from model Eq. (16) show that the values of velocity components are identical at the same point as is expected. However, the CPU times on IBM 360/91 by model Eq. (15) and (16) are 0.92 and 2.51 minutes, respectively. A saving of computer storage of about 150 K is achieved by model Eq. (16) though. Since the steady-state solution is sought, numerical scheme nos. 1 through 6 (Table 1) yield identical results as expected.

Freeze Transient Problem

A very small (6 x 3 m) laboratory-sized watershed was monitored by Freeze [10] to test his finite difference computer code. The same data were also used by Reeves and Duguid [4] to debug and test their finite-element model. These watershed data are again used in the present paper to compare model Eqs. (15) with (16).

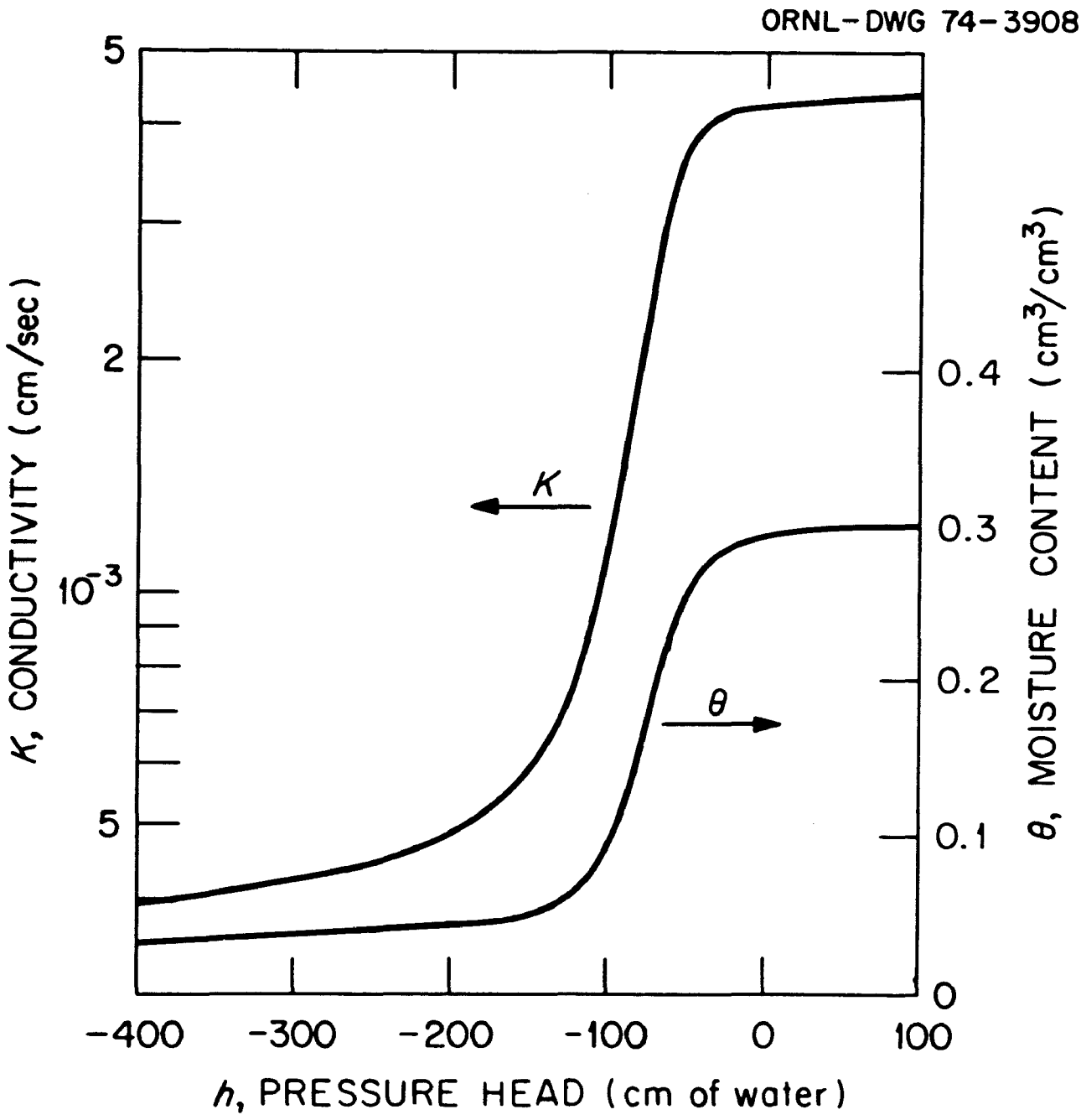

Fig. 3. Hydraulic conductivity and soil moisture characteristics of a hypothetical sandy soil.

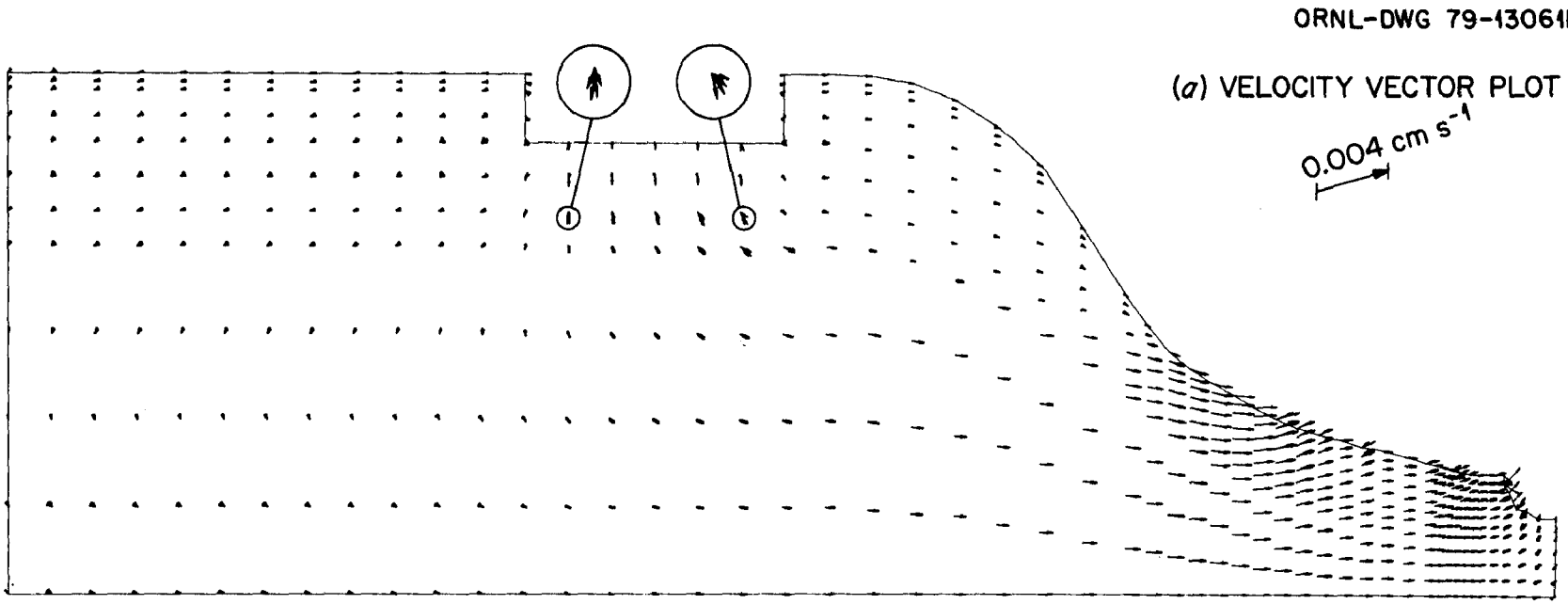

Fig. 4. Flow velocity plot as simulated by model Eq. (15) for the seepage pond problem.

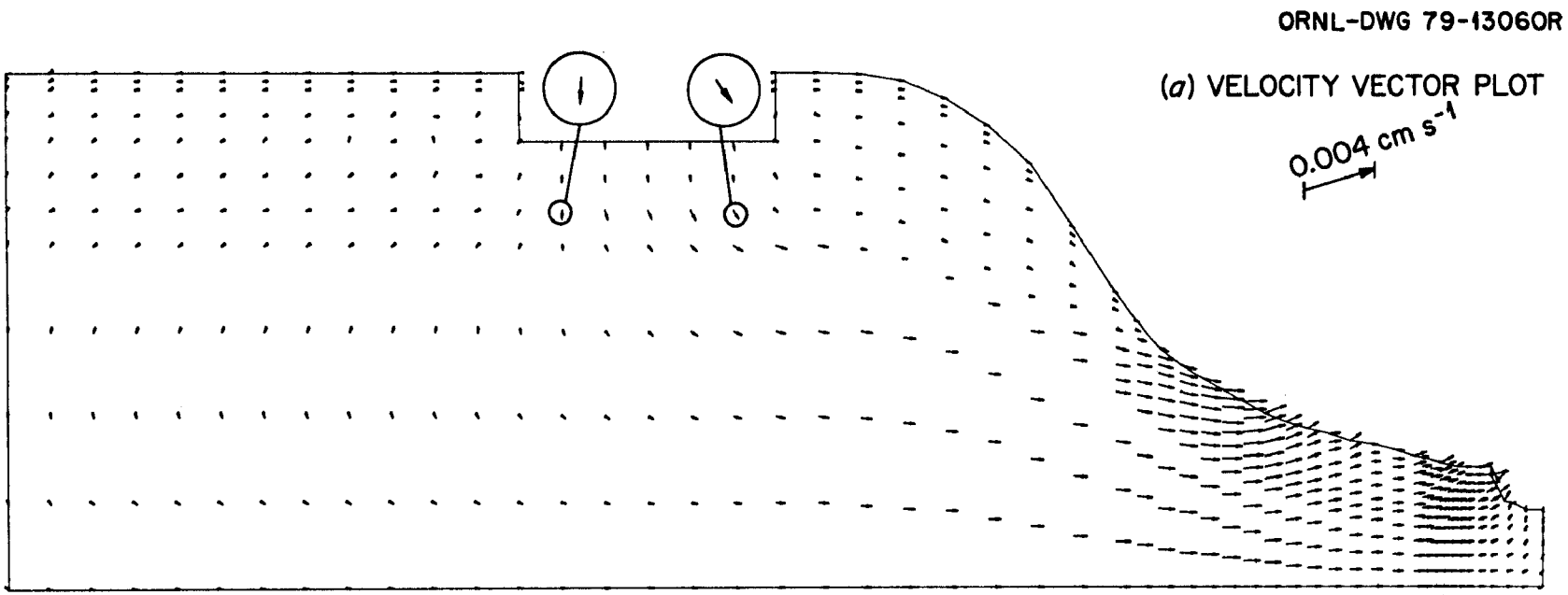

Fig. 5. Flow velocity plot as simulated by Model Eq. (16) for the seepage pond problem.

Table 2. Comparison of Velocity (cm/sec) Components Simulated by Model Eqs. (15) and (16), Respectively, at Three Selected Points

Node number	Element number	Model Eq. (15)		Model Eq. (16)	
		V_x	V_z	V_x	V_z
2	1	2.38E-8	-2.253E-8	1.24E-8	-4.44E-8
	2	2.33E-8	-6.54E-8	1.24E-8	-4.44E-8
179	152	2.26E-5	-9.15E-5	3.03E-5	-2.94E-4
	153	2.26E-5	-4.31E-4	3.03E-5	-2.94E-4
	159	3.31E-5	-9.15E-5	3.03E-5	-2.94E-4
	160	3.31E-5	-4.31E-4	3.03E-5	-2.94E-4
587	521	6.28E-5	1.85E-4	1.23E-5	1.84E-4
	522	6.28E-5	2.36E-4	1.23E-5	1.84E-4
	528	7.89E-10	1.85E-4	1.23E-5	1.84E-4

The flow system is shown in Fig. 6. It is composed of highly permeable sand, the unsaturated properties of which are shown in Fig. 3. To obtain initial conditions, pressure-head values were pre- scribed along the stream channel, part of the slope, and the upper plateau. Taking all other boundaries to be impermeable, a steady-state solution was determined which was the initial condition for the transient calculation.

Using Freeze's transient boundary condition (Figure 6b) and Reeves and Duguid's finite-element discretization #2 (Figure 6c), results obtained by models Eqs. (15) and (16), respectively, are shown in Figs. 7 and 8. Model Eq. (15) again displays the discontinuity of velocity vectors at all nodal points, while model Eq. (16) has completely eliminated this inconsistency. Furthermore, Table 3 shows that the mass balance has not been satisfied by model Eq. (15). At the end of about 3-h simulation time, the total net mass through all boundaries is only about 76.2% of the mass accumulated in the media as computed by numerical scheme no. 1 of model Eq. (15). In other words, 23.8% of the mass has not been accounted for, i.e., has been lost through boundaries. Reeves and Duguid [4] speculated that this large loss of mass might be eliminated by adding triangular elements. However, without using triangular elements, model Eq. (16) only yields a 2.2% mass loss by eliminating the discontinuity of the velocity and using Eq. (25) to evaluate the moisture rate change. An even larger mass loss of 29.7% is obtained by numerical scheme no. 2 of model Eq. (15). Model Eq. (16), on the other hand, renders a 3.6% mass gain. Thus, error of mass balance (positive for loss, negative for gain) by model Eq. (16) is much smaller than that by model Eq. (15). The CUP time on IBM 360/91 for models Eq. (15) and Eq. (16) are 2.3 and 4.5 minutes, respectively, but a saving of computer storage of about 140 K is obtained by the latter.

Table 3 also shows the percentage of mass change by all alternative numerical schemes. It is noted that the central difference standard Galerkin scheme in model Eq. (16) yields the best results. This is not surprising since the water transport equation does not contain advection terms.

CONCLUSION

A continuous velocity field is required for the simulation of waste transport in the subsurface aquifer system. The conventional approach used in finite-element modeling, that is, taking the derivative of the approximately computed pressure head field, results in discontinuity of velocity at element boundaries and nodal points. It may also yield large error in overall mass balance computation. Thus, it is imperative that the same finite-element method that is employed to simulate the pressure field be applied to Darcy's law to obtain the velocity field. This will ensure a continuous velocity field and greatly reduce the overall mass balance error. The central difference Galerkin scheme yields the lowest error, since the governing equation is basically the Laplacian type in spatial coordinates.

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• Comparison with FD Solution

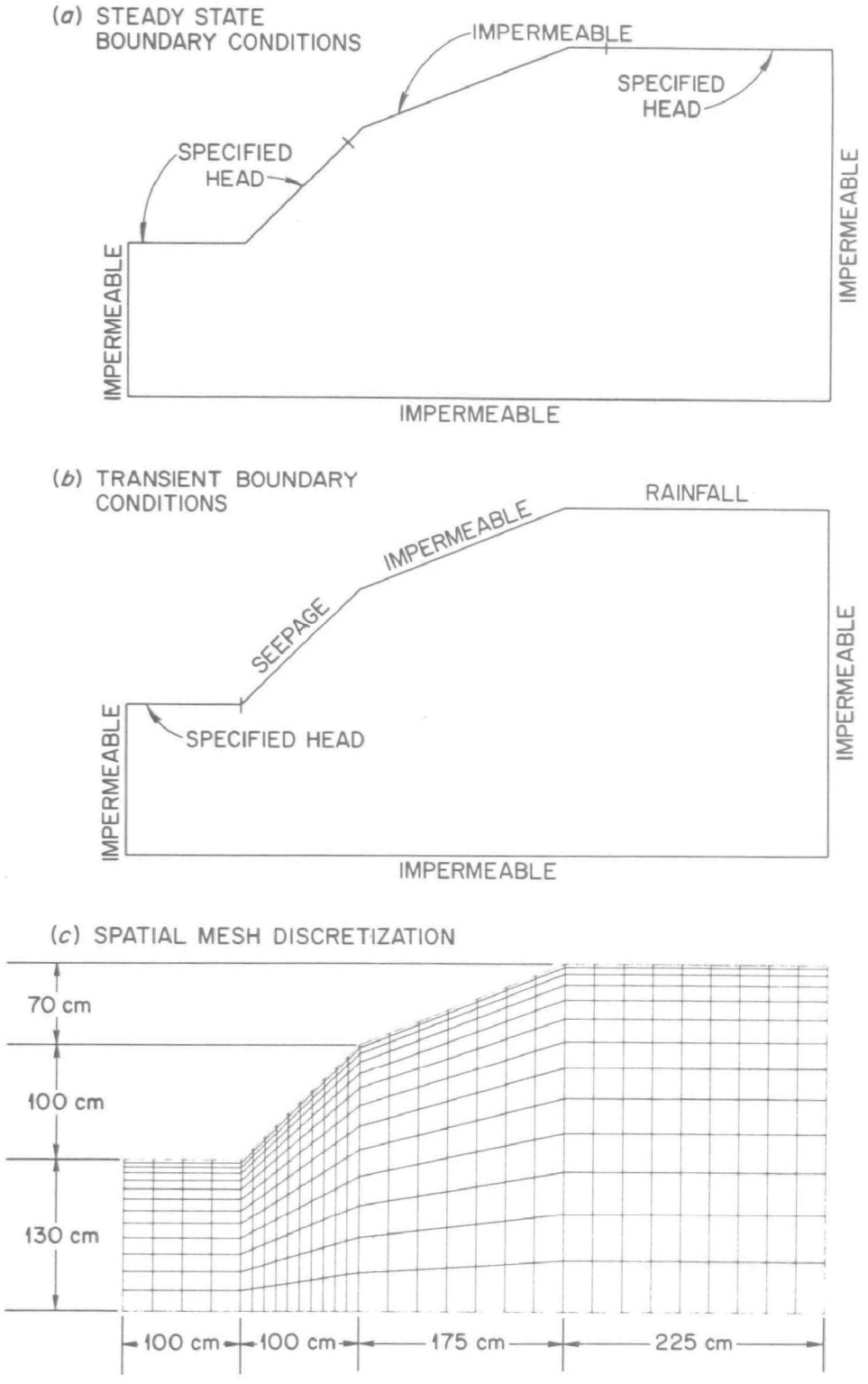

Fig. 6. Configuration of Freeze's experimental watershed: (a) steady state boundary condition, (b) transient boundary condition, (c) spatial finite element discretization after Reeves and Duguid (1975).

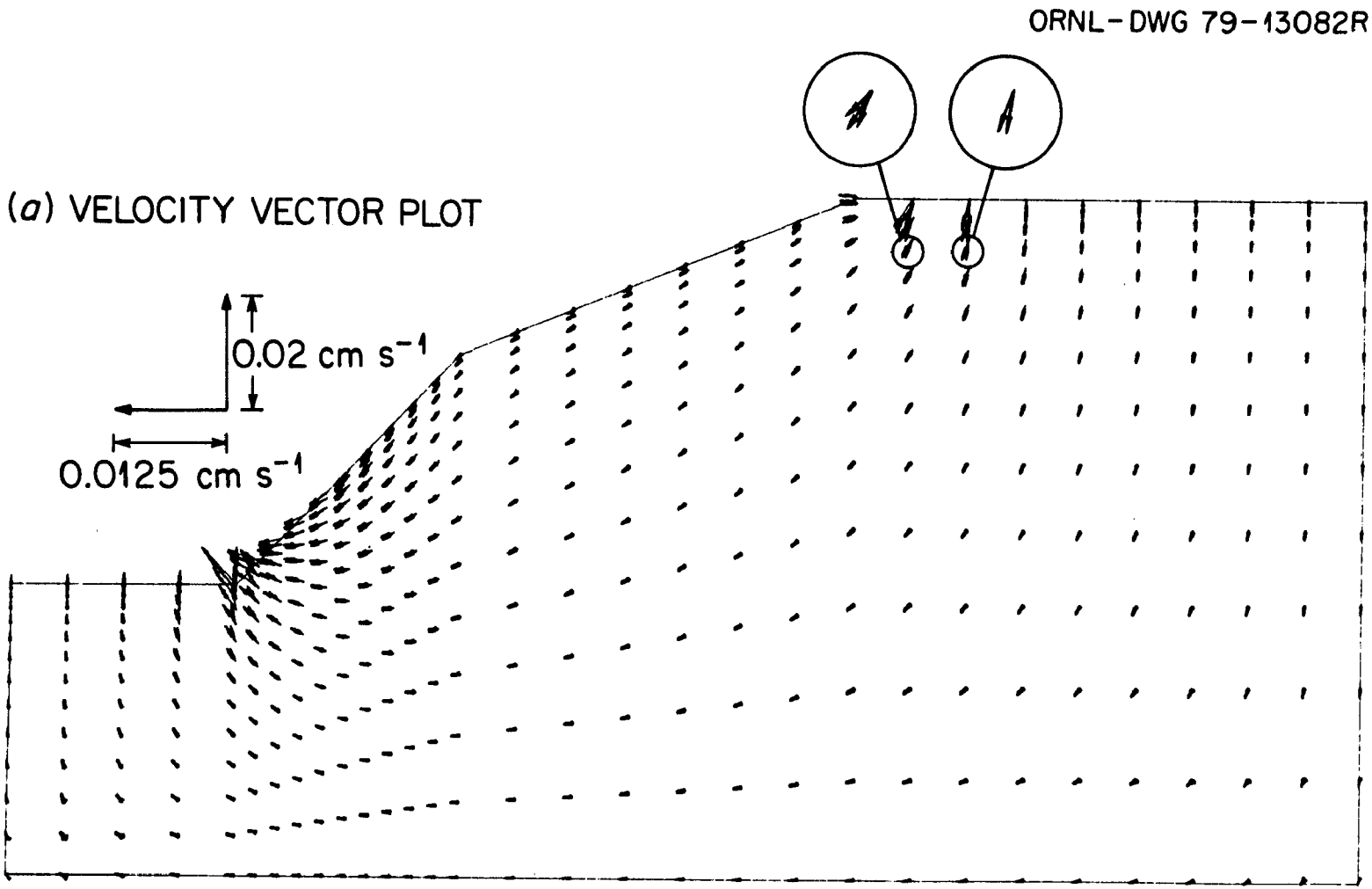

Fig. 7. Flow velocity plot at time equal to 2.96 h of Freeze's transient problem as simulated by Model Eq. (15).

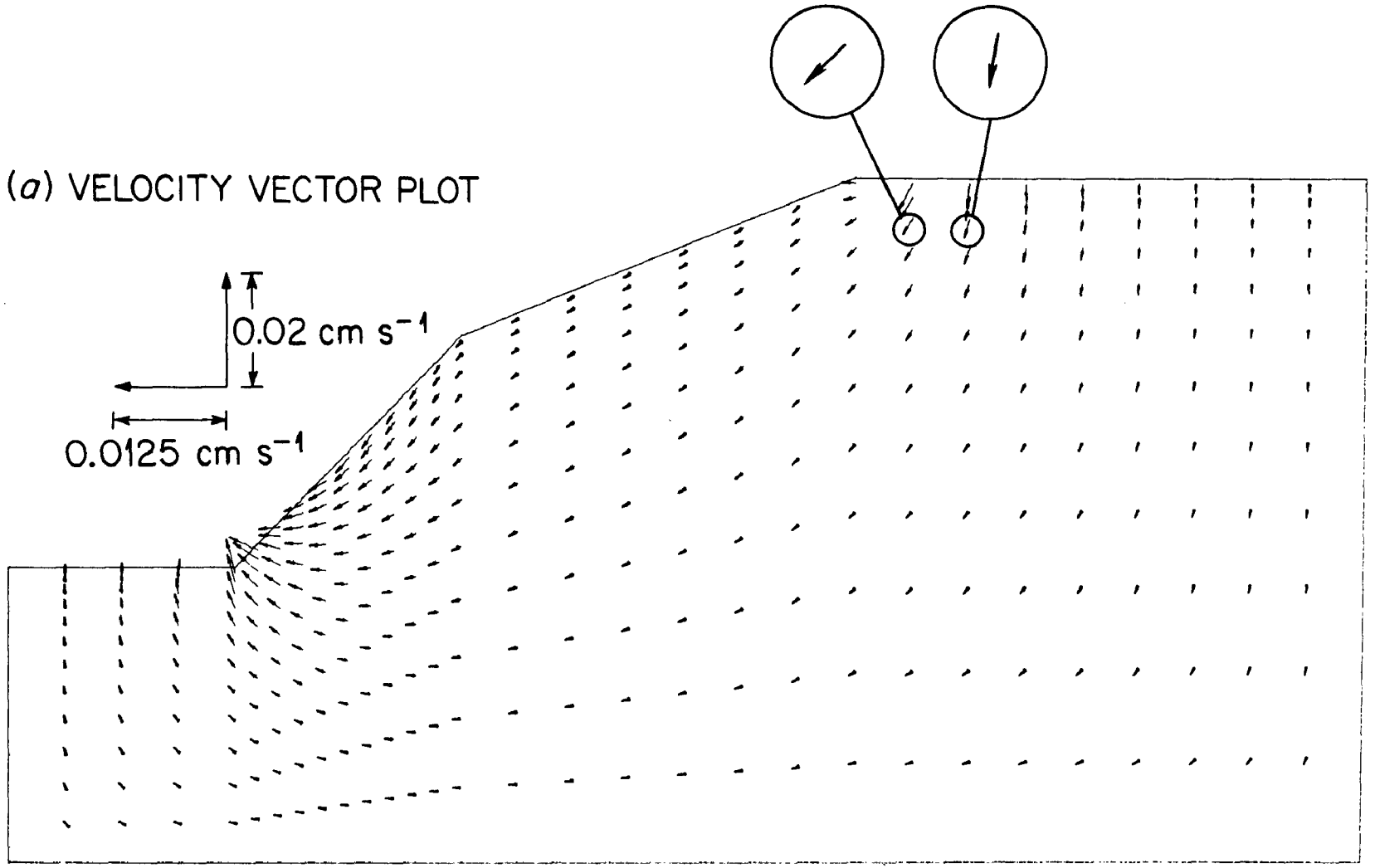

Fig. 8. Flow velocity plot at time equal to 2.96 h of Freeze's transient problem as simulated by Model Eq. (16).

Table 3. Comparison of Percentage of Mass Change of Freeze's Transient Problem as Simulated by Model Eq. (15) and (16)

	Scheme					
Model	1	2	3	4	5	6
Eq. (15)	23.8	29.7	N/A	N/A	N/A	N/A
Eq. (16)	2.2	-3.6	8.9	3.0	-3.2	-3.3

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FRACTURE FLOW MODELING FOR LOW-LEVEL NUCLEAR WASTE DISPOSAL

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ABSTRACT

Fracture flow modeling as applied to low level radioactive waste disposal sites is discussed. Low level waste disposal sites presently exist in fractured basalts, crystalline igneous rocks, and limestones. The primary objective of forecasting the migration of radionuclides from these sites requires the consideration of fracture flow modeling. Such modeling is also an integral part of the planning and analysis of field work at the site.

Fundamental mathematical models describing discrete fracture flow and equivalent anisotropic porous medium flow are reviewed. Consideration is given to the theoretical and field aspects of the problem of when and how to treat a fractured medium as an equivalent anisotropic porous medium. The input parameters required for each type of model are discussed.

Finally a brief description of some of the models developed at the Lawrence Berkeley Laboratory is given. The models include those based on the integrated finite difference, polygonal finite difference, and finite-element schemes.

INTRODUCTION

Fracture flow modeling is an attempt to consider the effects of discrete fractures in approximating the nature of fluid movement in a fractured medium. Fracture flow predominates whenever the fluid flux through the fractures is appreciably greater than that through the unfractured, porous matrix. This condition implies that the hydraulic conductivity of the fractures, whether completely open or partially filled, is substantially greater than that of the matrix. Fracture flow strongly influences groundwater particle flow velocities, flowpath directions and the mechanisms of sorption-desorption of migrating radionuclides, and thus is of considerable importance to the safe disposal of low-level nuclear waste within media where an interconnected network of open fractures exists. This paper discusses the fundamental principles of fracture flow and the circumstances under which fracture flow

must be considered in modeling low-level waste disposal sites. Brief descriptions of the various types of fracture flow codes available at LBL are given.

The most important fractured media in terms of existing low-level waste disposal sites are basalt, crystalline igneous rocks, and limestone. This is not to suggest that these rock types are the best for disposal or the most commonly occurring types of fractured media, but rather that many low-level waste sites have been constructed in them. Indeed, basalt and limestone are generally poor choices for containment and problems requiring remedial efforts are quite likely to occur at such sites unless they are properly designed for the existing fracture system. Matrix flow in each of these rock types is likely to be relatively small in comparison to the flow in the fractures.

The most obvious reason for the utilization of a model in studying a low-level waste site is to forecast the future migration of radionuclides from the site. There are, however, other reasons for employing a model that are just as important to the full assessment of the site. Because of the geologic and hydrologic complexities of most sites, the input parameters for forecasting the future of a site are generally difficult and costly to obtain. The availability of a model during the field phase of site assessment, when data for input parameters are being collected, can insure that the most useful information is collected in the most efficient manner. In particular, parameter sensitivity studies can be used to plan field work and provide assurance that characterization of some aspects is not being overemphasized to the neglect of others. Further, the availability of a model permits analysis of field test data, such as complex tracer tests, to an extent that would not be practical if only more conventional analytical techniques were available.

FUNDAMENTAL MATHEMATICAL MODELS

Flow through a fractured medium is generally mathematically described in one of three ways: (1) by considering each fracture as a discrete hydraulic conduit; (2) by assuming a hydraulically equivalent anisotropic porous medium and using the appropriate porous medium model; or (3) by a combination of (1) and (2).

Flow through a single fracture is normally represented by a parallel plate analogy [1]. If the flow is assumed to be laminar, the fluid single-phase and Newtonian, and the parallel plates smooth, the steady flux from a single fracture may be described by:

$$q = -\frac{(2b)^3}{12\mu}\rho g\frac{\partial h}{\partial \ell} \qquad (1)$$

where q = flux per unit length of fracture (L/T)
b = fracture half-aperture (L)
ρ = fluid density (M/L^3)
g = acceleration due to gravity (L/T^2)

μ = dynamic viscosity of the fluid (M/LT)
h = piezometric head (L)
ℓ = length along the fracture plane (L)

Utilizing the parallel plate analogy, it can be seen that the factor $(2b)^2/12$ in eq. (1) directly corresponds to the intrinsic permeability of a porous medium (k_{ij}). The extent of this correspondence is demonstrated in the following parallel development of the fundamental equations governing fluid flow and nonreactive solute transport in both porous media and fractures.

The equations governing flow in an anisotropic porous medium can be derived from continuity and Darcy's law and may be tensorially written as:

$$\frac{\partial}{\partial x_i} K_{ij} \frac{\partial h}{\partial x_j} + Q = S_s \frac{\partial h}{\partial t} \tag{2}$$

where K_{ij} = hydraulic conductivity tensor
$= \dfrac{k_{ij}\rho g}{\mu}$ (L/T)
Q = flow rate of source or sink per unit volume of rock (1/T)
S_s = specific storage (1/L)
t = time (T)
k_{ij} = intrinsic permeability tensor (L^2)

Along a fracture plane, consideration of continuity and eq. (1) requires that:

$$\frac{\partial}{\partial \xi_i} K^J \frac{\partial h}{\partial \xi_j} + m_i q_i \Big|_{\ell}^{u} = S_s^J \frac{\partial h}{\partial t} \tag{3}$$

where ξ_j = rectangular coordinates along the fracture plane
K^J = fracture hydraulic conductance
$= \dfrac{(2b)^2}{12\mu} \rho g$ (L/T)
S_s^J = fracture specific storage coefficient (1/L)
q_i = flow rate per unit volume of fracture across the fracture walls (1/T)
m_i = component of the unit vector outward normal to the fracture plane

The second term in the above equation refers to the difference between influx and efflux at the upper and lower fracture walls.

The equation governing the transport of a nonreactive solute in porous media is tensorially written [2]:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_i}(u_i C) = \frac{\partial}{\partial x_i} D_{ij} \frac{\partial C}{\partial x_j} + QC_{in} \tag{4}$$

where C = solute concentration (M/L^3)
u_i = seepage velocity in the ith direction (L/T)
D_{ij} = hydrodynamic dispersion tensor (L^2/T)
C_{in} = solute concentration at sources or sinks (M/L^3)

The velocities and coefficients of hydrodynamic dispersion are calculated from

$$u_i = \frac{K_{ij}}{\theta} \frac{\partial h}{\partial x_j}$$

$$D_{ij} = a_{ijkl} \frac{u_k u_l}{|u|} + \delta_{ij} D_d T_{ij} \qquad (6)$$

where a_{ijkl} = convective dispersivity tensor (L)
$|u|$ = seepage velocity magnitude (L/T)
D_d = molecular diffusivity coefficient (L^2/T)
T_{ij} = tensor of tortuosity
δ_{ij} = Kronecker delta
θ = effective porosity

Along a fracture plane the nonreactive solute transport equation can be written

$$2b \frac{\partial C}{\partial t} + 2b \frac{\partial u_i^J C}{\partial \xi_i} + \left(u_i C + D_{ij}^J \frac{C}{\partial x_j} m_i\right)\Bigg|_{\ell}^{u} = 2b \frac{\partial}{\partial \xi_i} D_{ij}^J \frac{\partial C}{\partial \xi_j} \qquad (7)$$

in which the third term refers to solute influx and efflux across the fracture walls. At present there exists no experimental data for D_{ij}^J, the hydrodynamic dispersion coefficient tensor. For approximation purposes, however, D_{ij}^J can be considered to vary from $D_d \delta_{ij}$ for a clean fracture to D_{ij} for a fully-filled fracture. Transport of reactive constituents can be treated by the source/sink terms in eqs. (4) or (7).

THE EQUIVALENT POROUS MEDIUM MODEL

A model based on only discrete fractures provides a theoretically correct flow pattern if all fractures and connections between fractures are considered. But, while such a model may be relatively easy to construct from a numerical point of view, the mass of input data required, the computational effort, and the difficulty of obtaining data for many real-world problems makes it generally difficult, if not impossible to apply to regional analysis.

One way to circumvent this problem is to represent the fracture system by an equivalent porous medium. An equivalent porous medium is a fictitious porous medium with material properties so selected that, under specific hydrologic and geometric conditions, the hydraulic behavior of the porous medium is in some respects the same as the hydraulic behavior

of the fractured rock. The validity of the equivalent porous medium concept is thus very site-specific and flowpath-specific. If it is assumed that for the purposes of the problem at hand, the domain being considered can indeed be represented by an anisotropic porous medium, then the major problem becomes that of determining the permeability tensor. The mathematics of calculating directional permeabilities from fracture orientation and aperture data based on the assumption that permeability is a function of aperture squared were first discussed by Romm and Pozinenko [3]. Extensive work in this area has been done by several others [1, 4, 5].

Under a general field gradient, flow in a single conduit may be described as [1]:

$$q_i = - \frac{(2b)^3}{12\mu} \rho g(\delta_{ij} - M_{ij}) \frac{\partial h}{\partial x_j} \tag{8}$$

where q_i = flow rate per unit width of the fracture plane in the jth direction (L^2/T)
δ_{ij} = Kronecker delta
M_{ij} = 3 x 3 matrix formed by direction cosines of the unit normal to the fracture plane
x_j = Cartesian coordinates (L)

It is further assumed that for a large number of fractures intersecting a sample line, each fracture has its image at a distance L equal to the length of the sample line and in the direction of the sample line. Thus, the spacing between the fracture and its repetition is given by [6]:

$$w = L|n_i D_i| \tag{9}$$

where w = spacing between fractures (L)
L = length of sample line (L)
n_i = component of unit normal to fracture plane
D_i = component of sampling line direction

The effective intrinsic porous medium permeability of a fracture is then given by:

$$k_{ij} = \frac{2}{3L} \frac{b^3}{|n_i D_i|} (\delta_{ij} - M_{ij}). \tag{10}$$

The equivalent permeability of the medium at a given sampling station is obtained by summing the contributions from the individual fractures. Where more than one station is used, the average of all stations is calculated. Knowing the permeability tensor, its principal components and directions may then be calculated.

This approach assumes that each fracture completely penetrates the volume being characterized, without changes in aperture or orientation.

Since in nature many fractures are observed to terminate over relatively short distances, this model would generally be expected to overestimate rock mass permeability.

If a similar procedure is followed to determine D_{ij} based on field data, then the anisotropic porous medium model described by eqs. (2) and (4) may be used directly.

In some cases where a relatively small number of large fractures exist together with a large number of small fractures with different orientation, it may be useful to employ both the discrete fracture and porous medium models. The equivalent tensorial properties would be applied to that portion of the medium dominated by the smaller fractures and the problem would be treated as a fractured anisotropic porous medium. Eqs. (2), (3), (4), and (7), and consideration of continuity would govern the system.

MODELING OF A FIELD SITE

Selection of a model for a particular field application requires two primary considerations. First, the type of output required of the model must be clearly defined, and second, the type of input available for the model from the field site must be identified. Put in another way, the data needs for decision-making that are to be supplied to the model must be compatible with the capabilities of the model, which in turn must be compatible with the physical and economic realities of obtaining the necessary data from the field and operating the model. Clearly, the output needs, the choice of model, and the input needs are all interdependent.

The types of output parameters required of models for safe disposal of nuclear waste will involve dose rates and contaminant concentrations under environmental conditions to be prescribed by the Environmental Protection Agency. Our purview as earth scientists will be to recommend the most appropriate approaches to obtaining the required information. This means balancing the applicability of models against the availability of input parameters to best achieve the output requirements.

Groundwater movement and nuclide transport in fractured media can be modeled with either a discrete fracture model or an equivalent porous medium model. The types of input parameters that are required for these two models are not the same. The fracture model requires fracture geometry data such as fracture orientation, spacing, and aperture while the porous medium model requires the large-scale averaged parameters of permeability and dispersion.

The question of which model to use for a given field site is, in general, not a simple one. The limitations of each model must be evaluated, and its applicability with regard to the model output requirements must be determined. From a theoretical point of view, the choice of models is generally a question of scale. If the representative elementary volume [2] concept is valid for the site, and if both the size of the site and the

scale of required output parameters are larger than the representative elementary volume, then the anisotropic porous medium equivalent can be employed. The other extreme of a case where there are a rather small number of identifiable distinct fractures within the entire site, calls for a discrete-fracture model. Both types of models suffer from difficulties in acquisition of input data. Parameters suitable for equivalent porous medium models must be obtained from field tests designed to average the individual effects of many fractures over volumes larger than the representative elementary volume. On the other hand, parameters suitable for discrete-fracture models must accurately identify the specific geometry of the principal flowpaths. Unfortunately, many near-surface low-level waste field sites will probably not clearly fit into either category and a hybrid model may be required.

In principle, the most straightforward method for determining the size of the representative elementary volume is to perform hydrologic tests in different portions of the site starting with small-scale tests (i.e., closely-spaced wells) and expanding the scale of each of the tests in increments. As the tensors of permeability and dispersion, computed from tests of progressively increasing scale, approach some type of consensus in magnitude and orientation at a particular test site, it could be assumed that the scale of the individual test at that particular location is approaching that of the representative elementary volume at that location. Further, if the results of the individual tests at different locations are seen to converge, then it could be concluded that the site as a whole can be described as a single anisotropic porous medium with similar properties throughout.

While this procedure appears to be straightforward, it may be impractical for many real-world problems. First, the procedure might be costly and time-consuming. Second, most field sites are likely to be heterogeneous, implying that this procedure would have to be performed for each fractured geologic formation at the site. Finally, determination of tensorial properties in the field, particularly for a three-dimensional case, would be quite difficult. Despite these difficulties, the alternative of measuring the geometry of all significant discrete fractures is likely to be impossible over any reasonably-sized field site, leaving us with little choice but to employ an equivalent porous medium model or a hybrid model at many sites.

An alternative to the direct large-scale field measurement approach described above is to compute equivalent porous medium properties based on many individual measurements of single fractures, using a procedure similar to that proposed by Snow [1] and discussed above. An extensive field evaluation of this approach is now being conducted by LBL at the Stripa test station in Sweden, and the results will be compared with those of a large-scale test involving 10^5 to 10^6 m^3 of rock [7].

For the modeling of a real field site, it may be best to not decide on the type of mathematical model to be used until substantial field data are available. Information on discrete fractures will be required in the design of field tests and in evaluating the applicability of the equivalent

porous medium concept, thus the field work will of necessity provide input parameters for both equivalent porous medium and discrete fracture models. Such an approach will provide more flexibility and will ultimately result in a better understanding of the site. After, and to a certain degree during the field-work phase of the study, both types of models, together with a hybrid having both discrete fractures and equivalent porous media, can be tried and the best model identified.

From a practical point of view the need for fracture data will require the addition of a limited number of activities to those required for the standard porous medium type characterization and assessment of a low-level site. In particular, fracture mapping and fracture core logging will have to be added to the geologic activities. Hydraulic and tracer testing will have to be performed in a somewhat more complicated fashion so as to test individual fractures. Finally, preparation of two or three types of mathematical models will be required.

MODELS AT LAWRENCE BERKELEY LABORATORY

The Lawrence Berkeley Laboratory is presently using three types of numerical models that have application to the modeling of low-level waste deposit sites. The first group of models is based on the integrated finite difference scheme. Examples of these programs are TERZAGHI [8], CCC [9], and SHAFT79 [10]. Of these, TERZAGHI may be the most useful for low-level site modeling. It solves a nontensorial form of eq. (2) in three dimensions. It has been used to model discrete fractures and some types of anisotropic porous media. It also has the capability to deal with one-dimensional consolidation.

The second group of models is based on the polygonal finite difference scheme. Examples are BIFDA and GENIE [11]. These models solve a three-dimensional form of eqs. (2) and (4). They can be used to deal with both discrete fractures and anisotropic porous media. In addition, they can handle heat transport.

The third group of models is based on the finite-element scheme. Examples of these models are ROCMAS [12]. FRACFLOW [13], and LINE ELEMENT [14]. These programs solve various forms of eqs. (2), (3), (4), and/or (7), for two-dimensional cases. The first two can be used for either discrete fractures or porous media. In addition, the first and second can deal with the effects of stress and the second can also deal with heat and anisotropic problems. The third program is a steady state line element code presently being used in research on the definition of the permeability tensor in random systems of discrete fractures.

The first group of models evolved from a coupled fluid-heat flow model. The second group was developed to provide good chemical transport and anisotropic media capabilities while maintaining three-dimensional capabilities. The third group was developed to deal specifically with discrete fractures with stress-dependent properties.

ACKNOWLEDGEMENTS

Work performed under the auspices of the U. S. Department of Energy through Lawrence Berkeley Laboratory, University of California, under contract W-7405-ENG-48.

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A CONCEPTUAL ANALYSIS OF THE GROUNDWATER FLOW SYSTEM AT THE MAXEY FLATS RADIOACTIVE WASTE BURIAL SITE, FLEMING COUNTY, KENTUCKY

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ABSTRACT

The complex groundwater system at the Maxey Flats radioactive waste burial site in Fleming County, Kentucky was investigated with the aid of a highly simplified, steady state, groundwater flow model. An analysis of the local hydrogeology suggests that at least two saturated groundwater flow systems are present at the site: a lower system in the bottom part of the Ohio Shale, and an upper, perched system extending from the base of the Bedford Shale up to a water table in the weathered part of the Nancy Member of the Bordon Formation. Unsaturated conditions may also exist in the Sunbury Shale. Simulations indicate that most of the water which recharges the upland surface of Maxey Flats is eventually discharged as seepage along the hillside through the upper part of the Farmers Member of the Bordon Formation and the Sunbury Shale.

INTRODUCTION

This report discusses the groundwater flow system at the Maxey Flats radioactive waste burial site in Fleming County, Kentucky. The groundwater system at Maxey Flats is complex; flow occurs mainly through fractures in hydraulically "tight" shales and sandstones. In addition, water levels from wells at the site indicate the possibility of unsaturated conditions at depth. At the present time the available data do not warrant a detailed model of groundwater flow; however, careful examination of the hydrogeology and the hydrologic setting of the site can help provide a conceptual understanding of the groundwater system.

Maxey Flats is topographically an isolated knob located in the Appalachian plateau region of eastern Kentucky. The Maxey site is located on one part of this knob and is bounded on three sides by streams (fig. 1). Relief between the upland surface and bordering valley bottoms is about 300 feet.

Maxey Flats is underlain by fractured shales and sandstones which dip gently (25 to 40 feet per mile) toward the southeast. The rock units

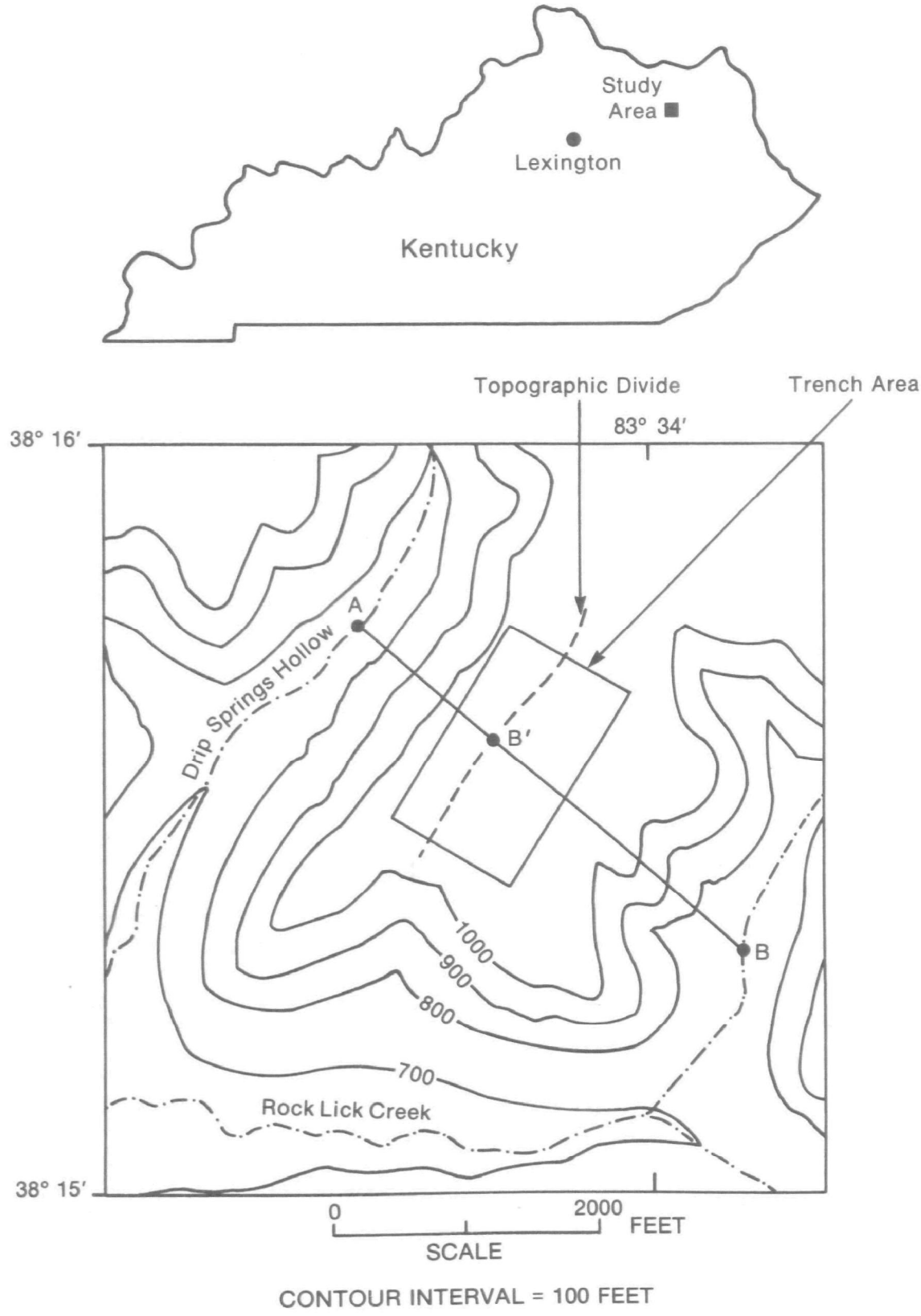

Fig. 1. Generalized topographic map of Maxey Flats, Fleming County, Kentucky.

directly underlying the Maxey Flats site are the Nancy and Farmers Members (predominantly a shale and sandstone respectively) of the Mississippian Bordon Formation, the Henley Bed (shale) of the Farmers Member, the Mississippian Sunbury Shale, the Mississippian and Devonian Bedford Shale, and the Devonian Ohio Shale, plus the upper part of the Silurian Crab Orchard Formation (shale). In this report, the Nancy and Farmers Members will be referred to as the Nancy shale and Farmers sandstone, and the Henley Bed will be referred to as the Henley shale.

The weathered and unweathered Nancy shale are separated by a thin (1 to 2 foot thick) sandstone bed, which is present over most of the site. This bed will be referred to as the sandstone marker bed. The upper part of the Farmers sandstone is a sequence of alternating, thin (1 to 3 foot thick) sandstone and shale beds, whereas the lower part of the unit is predominantly sandstone. The two parts probably have different hydraulic characteristics so, in this report, they are separated into the upper and lower Farmers sandstone. Figure 2 is a generalized geologic section taken along line A-B, shown in figure 1. Radioactive wastes were buried in trenches excavated in the Nancy shale on the upland surface.

The distribution of wells at Maxey Flats is shown in figure 3. E-wells were drilled by Emcon Associates. UA-wells, northeast of the burial area, and UB-wells, in the trench area, were drilled by the U.S. Geological Survey in 1976 and 1977. Well construction and water-level data are summarized in figures 4 and 5.

ANALYSIS

Conceptual Model

Eleven hydrogeologic units are exposed at Maxey Flats. The sequence of units, from top to bottom, and their thicknesses in feet, are:

1. Colluvium, which partially covers the hillsides (0 to 5)
2. Weathered Nancy shale, which covers the hilltops (1 to 25, with an average of about 20)
3. Sandstone marker bed, which is usually at the base of the weathered Nancy shale (1 to 2)
4. Unweathered Nancy shale (20 to 40, with an average of about 25)
5. Upper Farmers sandstone (15 to 20)
6. Lower Farmers sandstone (15 to 20)
7. Henley shale (7)
8. Sunbury shale (20)

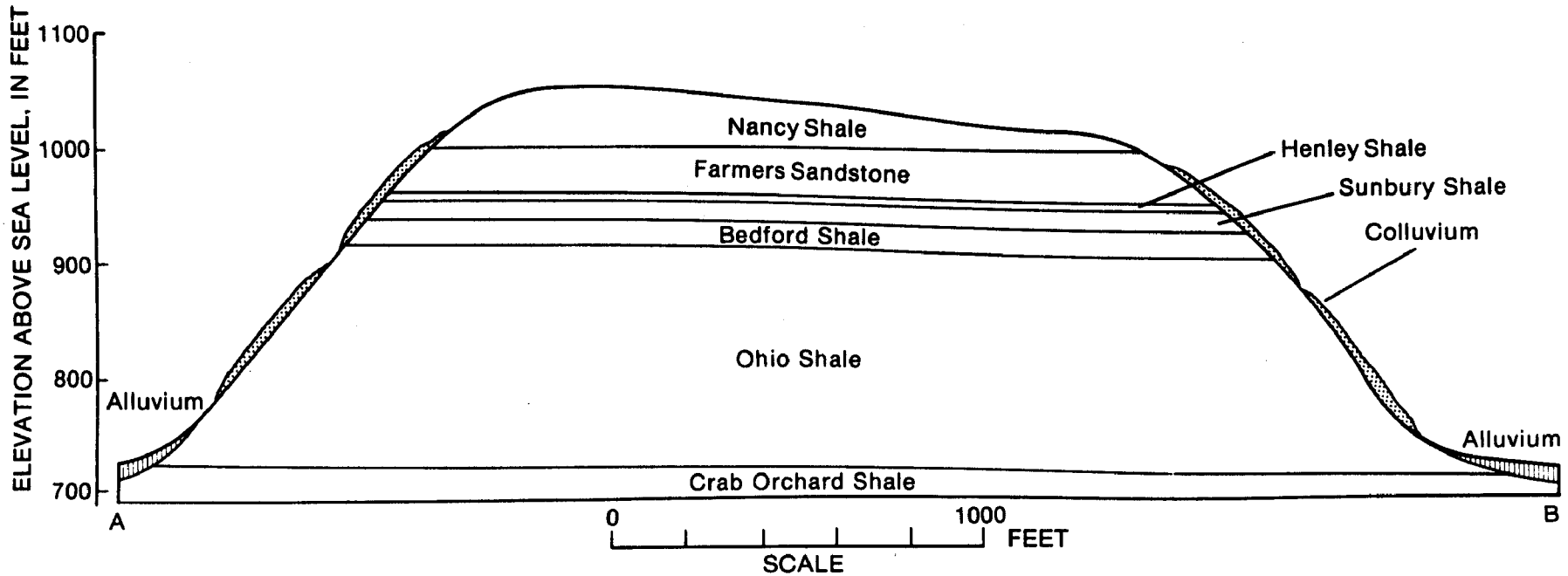

Fig. 2. Geologic section along line A-B in figure 1.

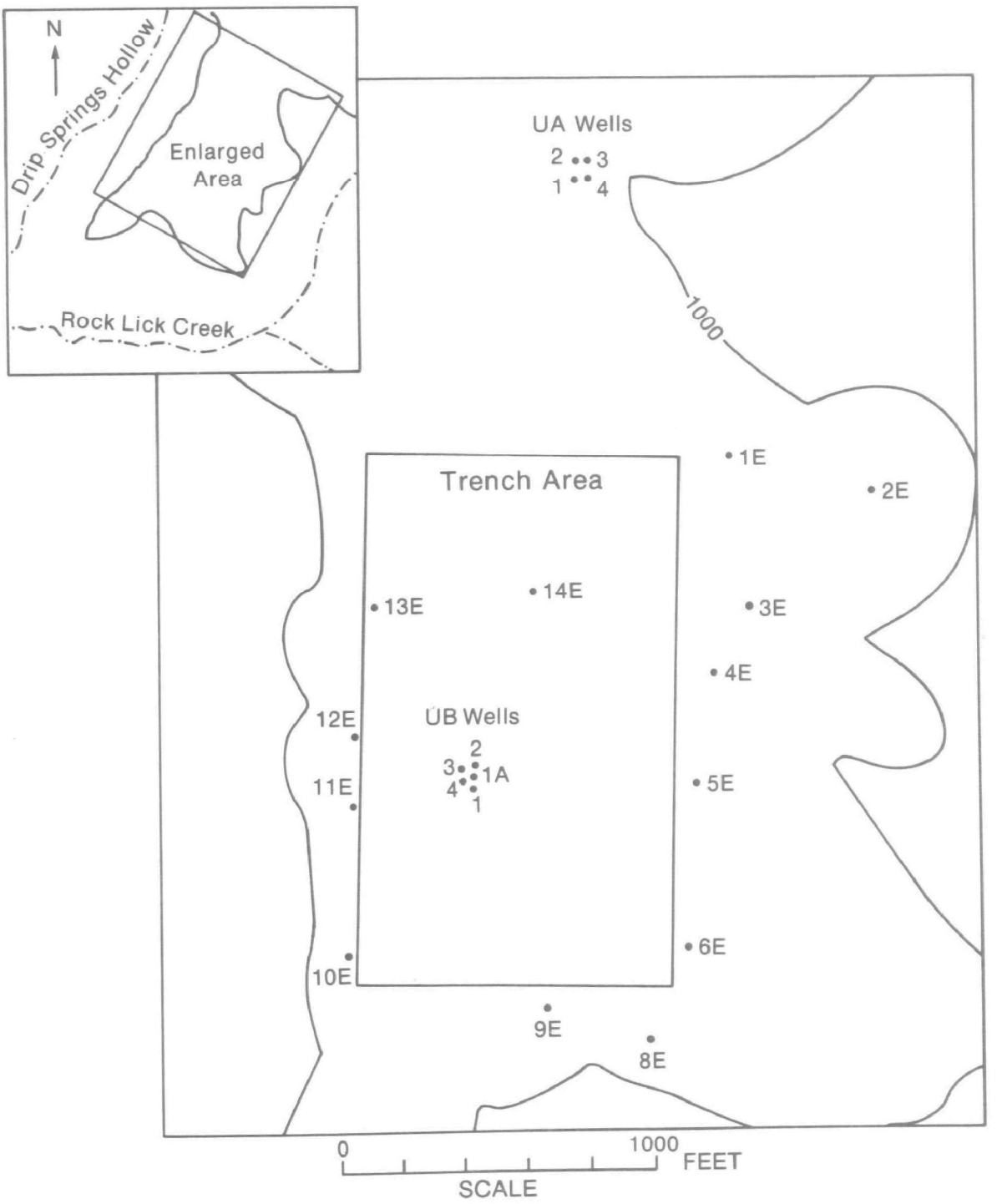

Fig. 3. Location of wells.

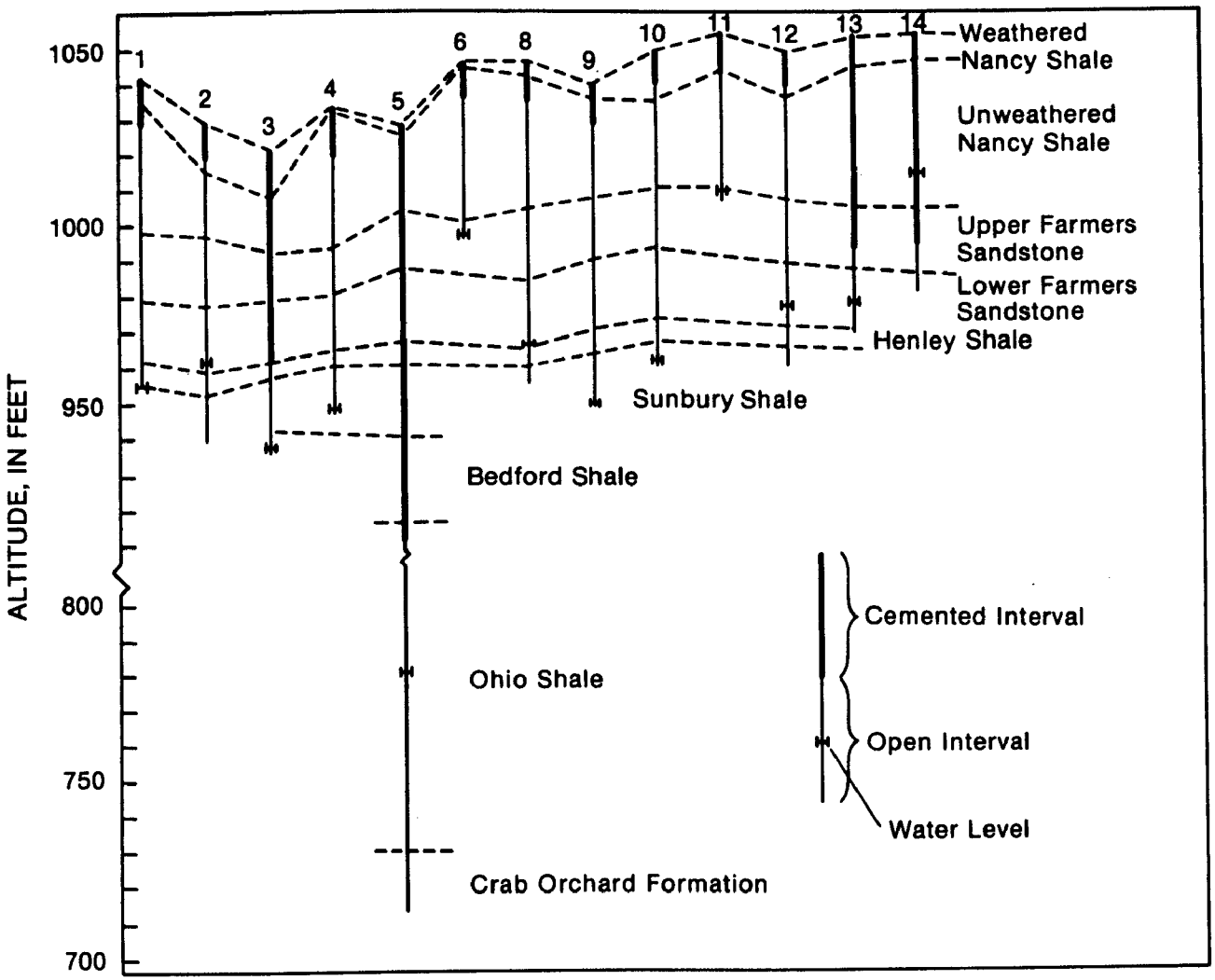

Fig. 4. Well construction information and water level data for wells drilled by Emcon Associates.

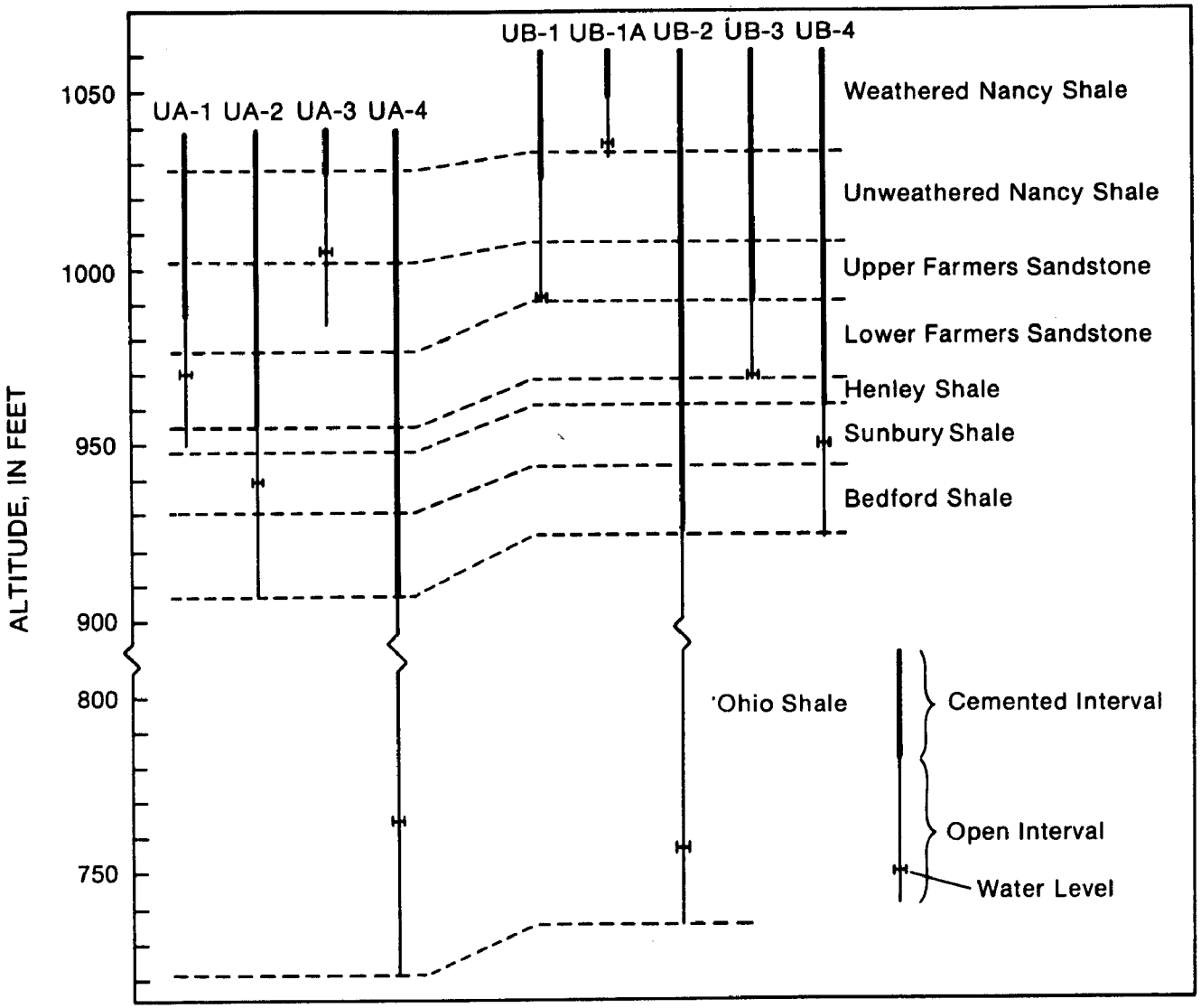

Fig. 5. Well construction information and water level data for wells drilled by U.S.G.S.

9. Bedford shale (20)

10. Ohio Shale (185)

11. Crab Orchard Formation, with only the upper few feet exposed in the valley bottoms (approximately 120)

No quantitative data are available regarding hydraulic properties of these units. Qualitative, visual observations of some properties (including porosity, fracture density, and groundwater discharge) were made at outcrops. The hydrogeologic units above the valley bottoms are grouped into four categories, based on visual observations and water-level recovery rates in wells finished in some of the units (Table 1). The colluvium is not considered in this study. It undoubtedly plays a role in controlling seepage along the hillsides; however, because there are no wells on the hillsides, the groundwater regime in the colluvium is unknown. The hydrogeology of Maxey Flats can be thought of as a series of extremely poorly permeable rock units alternating with a few layers of somewhat higher permeability. The upper part of the Crab Orchard Formation, which crops out in the valley bottoms, is a clayey shale with very few fractures; in this report, it is considered to be the "impermeable" base of the flow system.

The only significant groundwater flow at Maxey Flats occurs through fractures spaced from 1 to 40 feet apart. One way of modeling flow through fractured rock is to treat the fractured rock mass as a porous medium. That is, instead of distinguishing individual fracture-flow pathways, each point in the rock mass is assigned an hydraulic conductivity which represents a measure of the "average" water-transmitting ability of the fractures in the vicinity of that point. Fractured rocks appear to behave as porous media on a scale where the distance between fractures is small compared with the dimensions of the flow system being considered. Fractured rocks are usually treated as porous media for regional flow studies, but for some small-scale studies (such as dam site investigations) it is sometimes necessary to consider flow through a network of discrete fractures (e.g., Wilson and Witherspoon, 1970). The major drawback with fracture-network flow models is that they require detailed information about the spatial distribution and hydraulic properties of individual fractures which is rarely available. In the case of Maxey Flats, it is probably possible to obtain an adequate representation of the head distribution in the fracture network by assuming porous media flow; however, it may be very difficult to measure the head distribution in the fracture network. In fractured rocks that have extremely low intergranular permeability, the water level in a well may represent the head in a single fracture at the point where the fracture intersects the open interval. If more than one fracture intersects the well, the water level will represent a composite of the heads in the individual fractures at the points of intersection. Water level data from fractured rocks is therefore often difficult to interpret because the location of fracture intersections is usually not known.

Water levels from wells at Maxey Flats indicate a large decrease in head with depth. This fact has led previous workers to suggest that

Table 1. Qualitative classification of the hydrogeologic units

Medium	Hydraulic Conductivity		
	Low	Very Low	Extremely Low
Colluvium	Weathered Nancy shale, including the sandstone marker bed Sunbury Shale Ohio Shale	Unweathered Nancy shale Lower Farmers sandstone	Upper part of Crab Orchard Formation

Table 2. Distribution of discharge for the simulations illustrated in figures 7 and 8.

	Percent of Total Discharge		
	Upper Farmers sandstone	Sunbury Shale	Bedford Shale
Figure 7	60	37	3
Figure 8	66	23	11

unsaturated conditions may exist within as many as four hydrogeologic units: the Nancy shale, Farmers sandstone, Sunbury Shale, and the Ohio Shale (Papadopulos and Winograd, 1974). Isolated lenses of saturation bounded above and below by unsaturated conditions can occur in sequences of rock which have layers of contrasting hydraulic conductivity. These lenses of saturation, often referred to as "perched" groundwater, form whenever a layer of relatively low conductivity (a confining bed) is unable to transmit enough water to maintain complete saturation throughout an underlying layer of higher conductivity which drains laterally. Seepage outflow along the hillsides tends to drain the more permeable layers and create a favorable situation for the occurrence of perched ground water zones, separated by drained unsaturated zones.

In theory, saturated-unsaturated flow models (e.g., Freeze, 1971) can accurately simulate the groundwater flow field for a hydrogeologic system containing perched groundwater. At Maxey Flats, however, the lack of data, especially with regard to the hydraulic properties of the unsaturated zones, precludes the use of a complicated saturated-unsaturated flow model. An obvious alternative is to treat each perched groundwater lense as a distinct, saturated flow system. The entire groundwater system can then be modeled by determining the flow field for each of the perched systems sequentially, from top to bottom, using the discharge from the basal confining bed in one system as recharge to the underlying system.

It is assumed here that the transition from saturated to unsaturated conditions occurs at the base of the confining bed, where the pressure is assumed to be atmospheric. It can be shown (Zaslavsky, 1964) that the pressure in the lower part of the confining bed will actually be slightly less than atmospheric, and that the lowermost part of the confining bed can even be unsaturated in certain situations. For the purposes of this study, however, the error due to neglecting these additional complications is small compared to the other uncertainties in the analysis.

It should also be noted that what is interpreted as an unsaturated zone in a confined layer may actually be a zone saturated at less-than-atmospheric pressure. In such a case, a well completed in a rock unit saturated partly with water at less-than-atmospheric pressure and partly with water at greater-than-atmospheric pressure would accumulate water only from that part of the unit at greater-than-atmospheric pressure. The water level in the well could therefore be far below the top of the saturated unit. For purposes of brevity, the upper part of such a unit will be referred to in this report as unsaturated, but it is understood that the "unsaturated" zone may actually be saturated, but partly at less-than-atmospheric pressure.

For an isolated hill such as Maxey Flats, the potential for a perched water table to exist within a confined layer increases as the contract in hydraulic conductivity between layers increases. Thick layers are also more likely to contain unsaturated zones simply because they require a greater inflow from the overlying confining bed to stay completely

saturated. Furthermore, because discharge may occur through seepage faces in each layer, inflow from above to successively deeper layers decreases; consequently, deep layers are more likely to contain unsaturated zones than are shallow layers of equivalent conductivity and thickness.

The Ohio Shale possesses many of the characteristics important for the development of unsaturated conditions; it is thick, has adequate permeability, and is located at a low stratigraphic position in the hill. There is, in fact, evidence that water table conditions probably do exist within the Ohio Shale. Three wells open to nearly the entire 185-foot thickness contain less than 50 feet of water. If the shale were completely saturated at greater than atmospheric pressure, these low water levels would indicate a large vertical head gradient, and therefore a large component of vertical flow. However, the Ohio Shale is underlain by the poorly permeable upper part of the Crab Orchard Formation; consequently, flow in the Ohio Shale (especially the lower part) should be nearly horizontal due to the high contrast in hydraulic conductivity. The most plausible explanation for the low water levels appears to be that the upper part of the Ohio Shale is unsaturated. At least two wells drilled in the Ohio Shale encountered isolated zones of water some 30 to 50 feet above the ultimate static water levels, which could indicate that there is actually more than one saturated zone within the Ohio Shale. There is no way to check this hypothesis, however, because all of the wells in the Ohio Shale are open to the entire 185-foot thickness.

The existence of perched water tables within the upper Farmers sandstone and the Sunbury Shale is problematical. Dry wells finished in these units probably fail to intersect water-bearing fractures, and others with extremely low water levels may intersect fractures only at deep levels. A number of wells do not have relatively high water levels, which suggests that the upper Farmers sandstone and the Sunbury Shale could be completely saturated. Due to its lower stratigraphic position in the hill, the Sunbury Shale is the more likely of these two units to contain an unsaturated zone.

Based on the preceding analysis, Maxey Flats could be considered to consist, conceptually, of two saturated flow systems: an upper system which extends from just above the sandstone marker bed down to the base of the Bedford Shale, and a lower system which occupies the bottom part of the Ohio Shale. Only the upper flow system is considered in detail because water level data is insufficient to warrant a model analysis of groundwater flow in the Ohio Shale.

Mathematical Model

Idealized, two-dimensional vertical cross-sectional flow models are useful tools for studying general conceptual features of complex flow systems. The governing equation for two-dimensional, steady-state groundwater flow is:

$$\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right) + \frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right) = 0 \qquad (1)$$

where K_{yy} and K_{zz} are the hydraulic conductivities in the horizontal and vertical directions, respectively, and h is the hydraulic head. For this report, equation 1 was solved numerically using a finite difference approximation.

A representative vertical cross section was taken through the central part of the hill and oriented perpendicular to the topographic divide (line B'-B in figure 1). Boundary conditions for the upper flow system are summarized in figure 6. The left boundary is considered to be a no-flow boundary corresponding to a groundwater divide near the center of the hill. Heads along the lower boundary are set equal to the elevation of the base of the Bedford Shale. Heads along the water table in the weathered Nancy shale are assumed to vary linearly from a value corresponding to the water level in well UB-1A near the center of the hill to a value equal to the elevation of the top of the sandstone marker bed at the edge of the upland surface. The seepage boundary along the hillside is slightly more complicated. As a first approximation, the head at each point along the hillside was set equal to its elevation. Equation 1 was then solved for the head distribution. Occasionally, some sections of the hillside showed an anomolous horizontal component of flow back into the hill, which indicates that the flow conditions within the system are unable to suport the heads specified along those parts of the hillside. These "back flow" regions were changed to be no-flow boundaries, and equation 1 was solved again. This procedure was repeated until no more anomolous "back flow" regions occurred. An iterative approach of this type is frequently used to model steady-state flow in systems which contain seepage faces (Freeze and Cherry, 1979).

DISCUSSION

Figures 7 and 8 present the results of simulations for two different conductivity distributions which reproduce the important features of the head distribution in the upper flow system at Maxey Flats. The flow system is characterized by nearly vertical flow in the three major zones of low hydraulic conductivity (the unweathered Nancy shale, the lower Farmers sandstone and Henley shale, and the Bedford Shale) and essentially horizontal flow in the upper Farmers sandstone and the Sunbury Shale. The presence of the unsaturated zone below the Bedford shale assures a large average vertical head loss in the upper flow system. In addition, the simulations demonstrate how a well such as 14E, located near the center of the hill and finished primarily in the upper Farmers sandstone, can have a water level far above the top of the upper Farmers sandstone, whereas similar wells located around the perimeter of the hill often have much lower water levels.

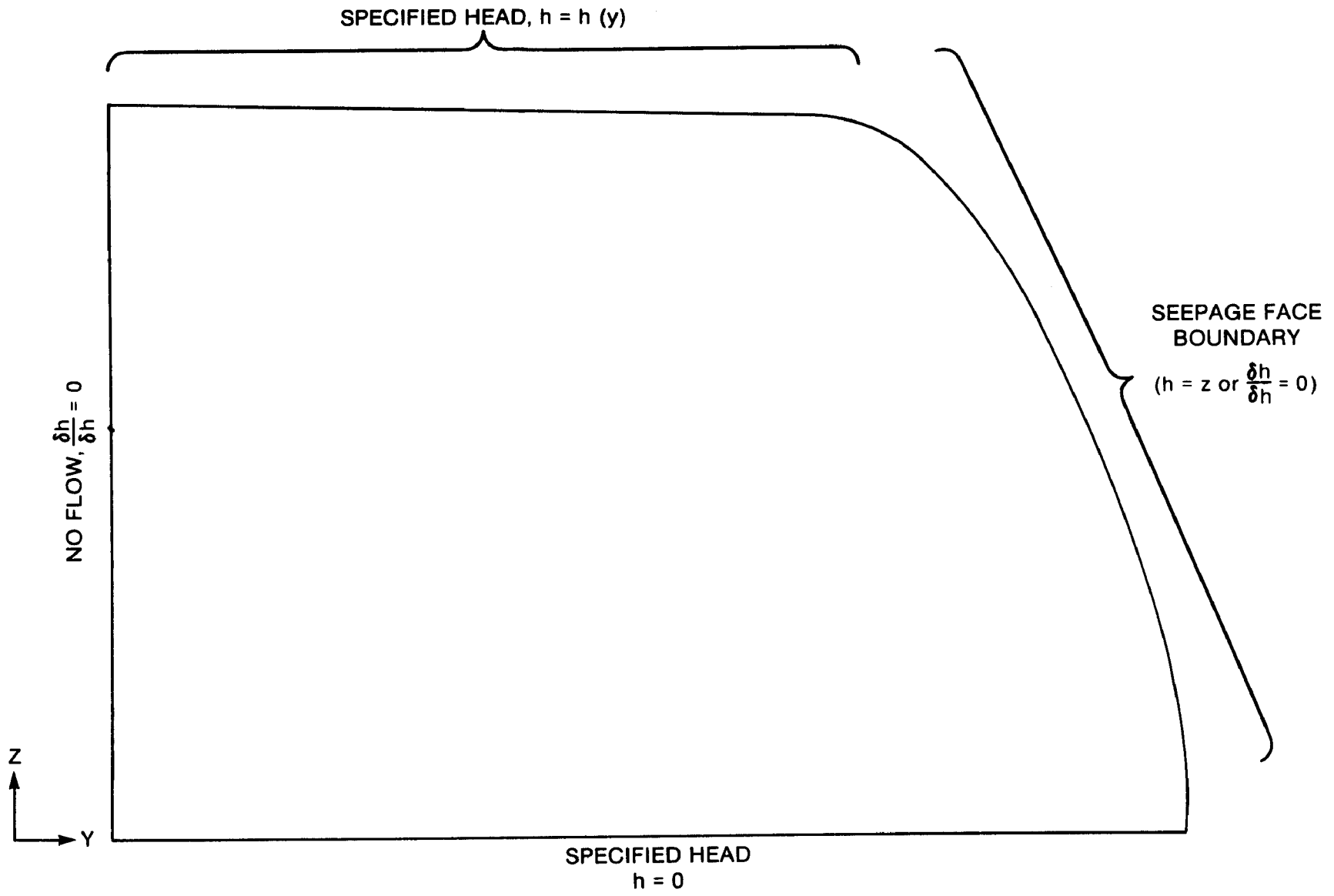

Fig. 6. Schematic diagram illustrating boundary conditions for the groundwater flow model.

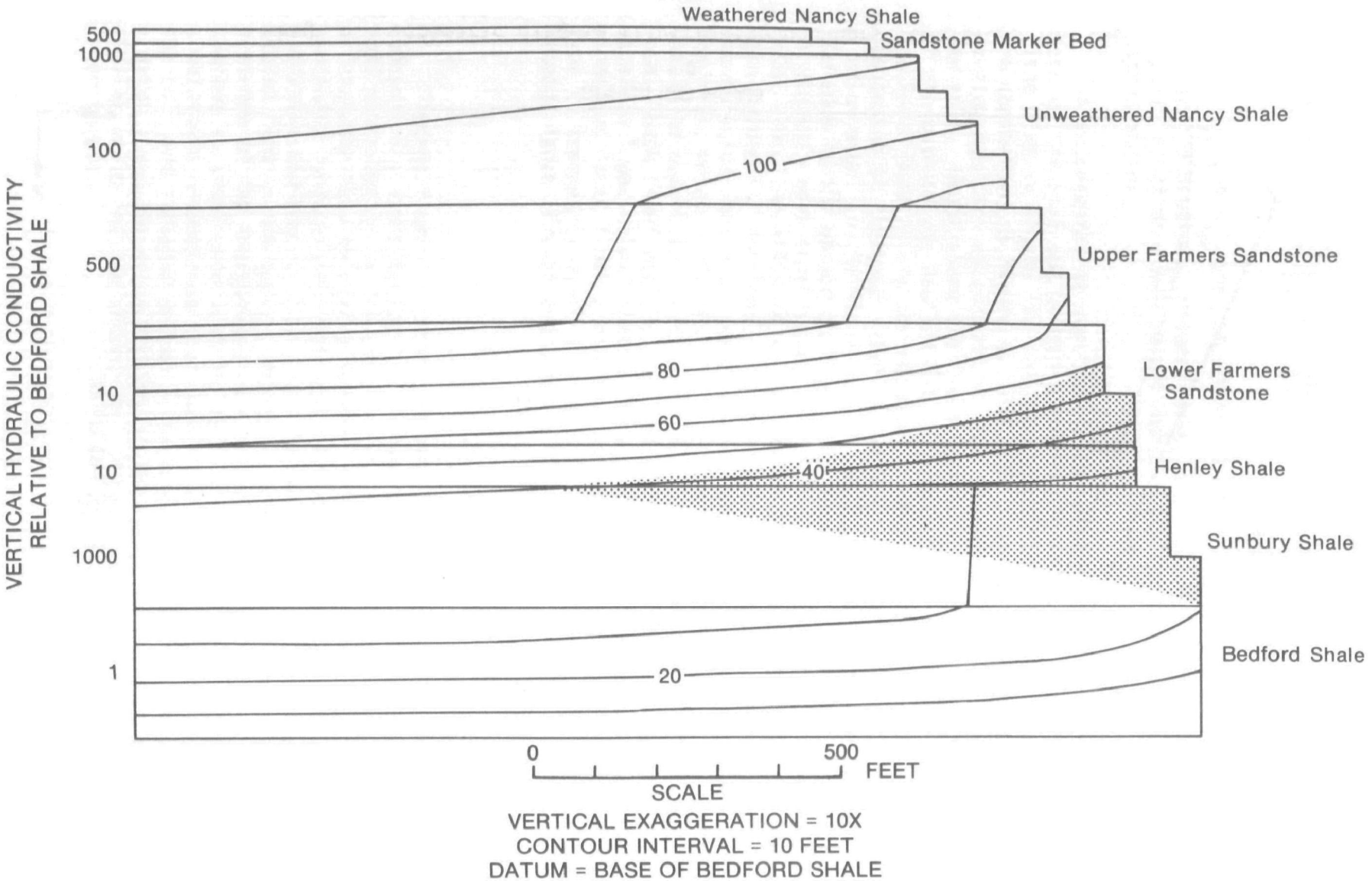

Fig. 7. Simulated head distribution for the relative conductivity distribution, 500: 1000: 100: 500: 10: 10: 1000: 1.

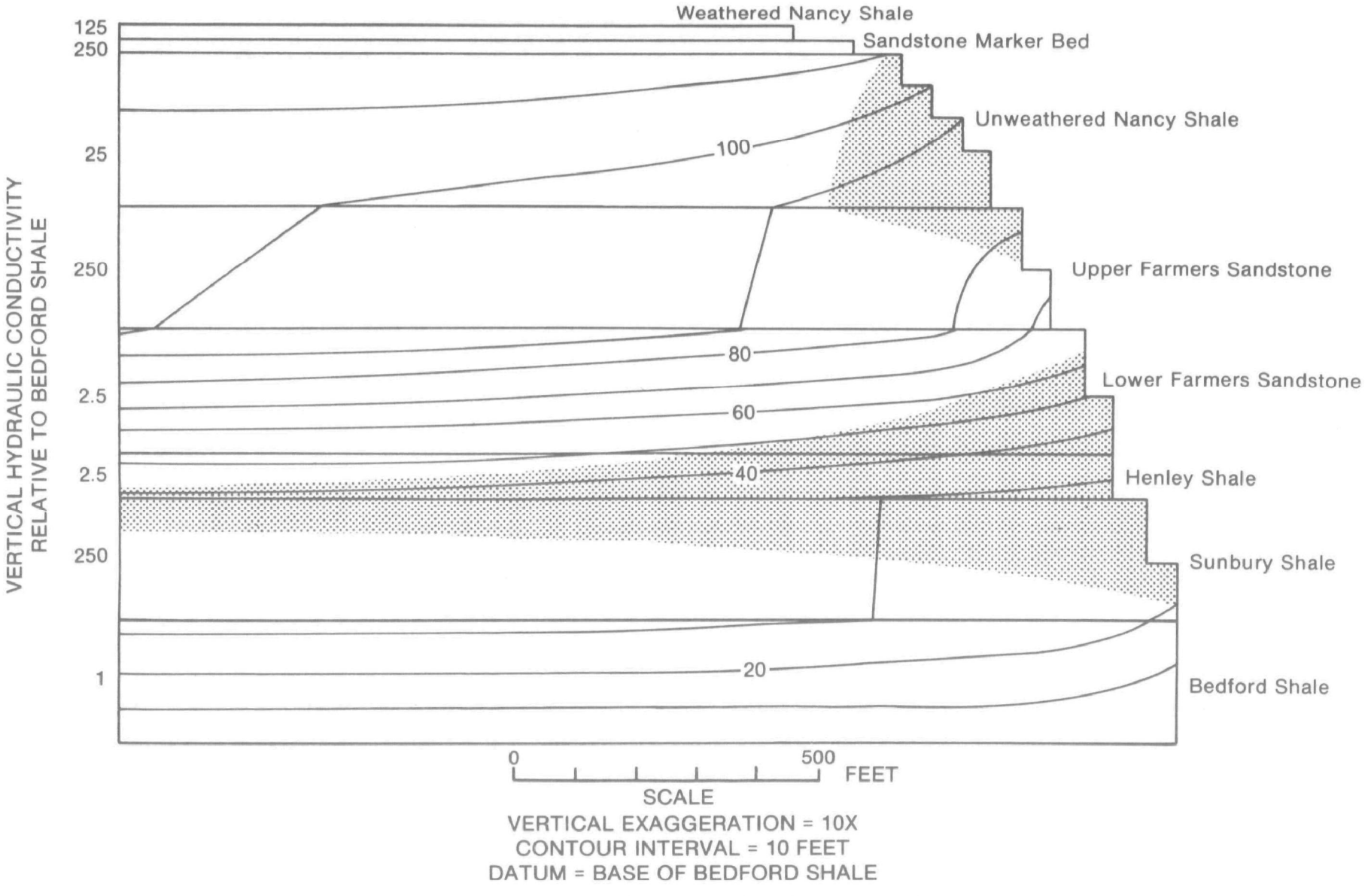

Fig. 8. Simulated head distribution for the relative conductivity distribution, 125: 250: 25: 250: 2.5: 2.5: 250: 1.

The shaded areas in figures 7 and 8 indicate regions where the predicted head is less than the elevation head; that is, regions where the pressure is less than atmospheric. Because rocks tend to become unsaturated when the pressure falls more than a few feet below atmospheric pressure, regions of sub-atmospheric pressure predicted by these simulations can be interpreted as an indication that unsaturated conditions could exist even though the model used in this analysis has no way of accounting for unsaturated conditions.

Figures 7 and 8 also illustrate two of many possible distributions of unsaturated zones. In figure 7, the upper flow system is completely saturated except, perhaps, for a small part of the Sunbury Shale and the overlying confining layers near the hillside. It is probably reasonable to assume that most of the more permeable units are unsaturated to some extent near the edge of the hill. In figure 8, the head everywhere in the Sunbury Shale is far below the top of the unit, which implies that water table conditions could exist throughout the Sunbury Shale. All that can be concluded, however, is that it is at least possible that water table conditions exist in the Sunbury Shale beneath the entire area of the hill.

Most of the water which enters as recharge to the upland surface of Maxey Flats in the two simulations discussed above is discharged along the hillside through either the upper Farmers sandstone or the Sunbury Shale (Table 2). It should be noted that the discharge distribution is a strong function of the anisotropy in hydraulic conductivity. For most of the simulations made during this study it was assumed that the horizontal conductivity was 100 times larger than the vertical conductivity due to the fact that fractures appear to be much more continuous in the horizontal direction than in the vertical. A few simulations were made which assumed isotropic conditions ($K_{yy} = K_{zz}$). In those cases, a much larger fraction of the groundwater flow (over 75 percent) discharged across the base of the Bedford Shale. However, the isotropic simulations were not able to account for the large heads in the upper Farmers sandstone.

The sandstone marker bed, one of the most permeable units at the site, occurs directly beneath the trenches; consequently, the possibility of radionuclide movement in the sandstone marker bed is of major concern. The models presented in this report cannot provide good, quantitative estimates of flow in the sandstone marker bed, but they do emphasize that the horizontal component of the hydraulic gradient in the sandstone marker bed should be essentially equal to the slope of the upper water table. Thus, in order to minimize horizontal flow in the sandstone marker bed it is extremely important to maintain low water levels in the trenches over the central part of the hill. In the simulations presented here most of the flow in the sandstone marker bed is downward into the underlying unweathered Nancy shale. Field data indicates that there is a significant component of horizontal flow of contaminated trench water in the sandstone marker bed.

This investigation illustrates the difficulty and complexity of defining the subsurface flow system in a layered, fractured-rock system of extremely low permeability. The basic constraint in modeling the system is the shortage of reliable field-measured parameters such as the horizontal and vertical hydraulic conductivities in all the major layers as well as the lack of adequate hydraulic head measurements. The model itself is capable of incorporating many different combinations of input parameters and boundary conditions. The results presented in this report do not necessarily approximate "actual" conditions in the field; they merely typify some possibilities based on qualitative estimates of hydraulic conditions at the site.

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COMPUTER SIMULATION OF GROUNDWATER FLOW AT A COMMERCIAL RADIOACTIVE-WASTE LANDFILL NEAR WEST VALLEY, CATTARAUGUS COUNTY, NEW YORK

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ABSTRACT

Commercial low-level radioactive wastes were buried in trenches excavated in a clay-rich till of low hydraulic conductivity near West Valley, N.Y., from 1963 to 1975. Groundwater from the trenches flows out laterally and downward through approximately 25 m of till.

A two-dimensional finite-element computer model was used to evaluate factors controlling groundwater flow in two vertical sections. Measured heads in 24 piezometers along these sections were most accurately reproduced by simulating four geologic units, each internally isotropic but differing in hydraulic conductivity to reflect fracturing near land surface and increased consolidation with depth. The model accurately simulated the changes in head that followed removal of water from one of the trenches. Specific-storage values required to calibrate the model for transient conditions agreed well with values derived from four consolidation tests of till samples.

Infiltration rates ranging from 3.8 centimeters per year near swampy areas to 1.5 cm/yr along scraped or smooth, sloping surfaces were used to simulate observed areal variation of head in the till. Simulations indicated that water flowing laterally out of a trench would not intersect nearby intermittent streams as long as the water level in that trench remained below the trench cover.

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INTRODUCTION

Location and Physical Setting

A State-licensed landfill for commercial radioactive wastes is among the facilities at the Western New York Nuclear Service Center, which occupies 13.5 km^2 (3,350 acres) in the northern part of Cattaraugus County, about 50 km south of Buffalo, N.Y. (fig. 1). The center is in a sparsely populated region of the glaciated Allegheny plateau (1) that is characterized by rounded hills of Devonian shale capped with thin deposits of till and separated by bedrock valleys containing as much as 150 m of drift.

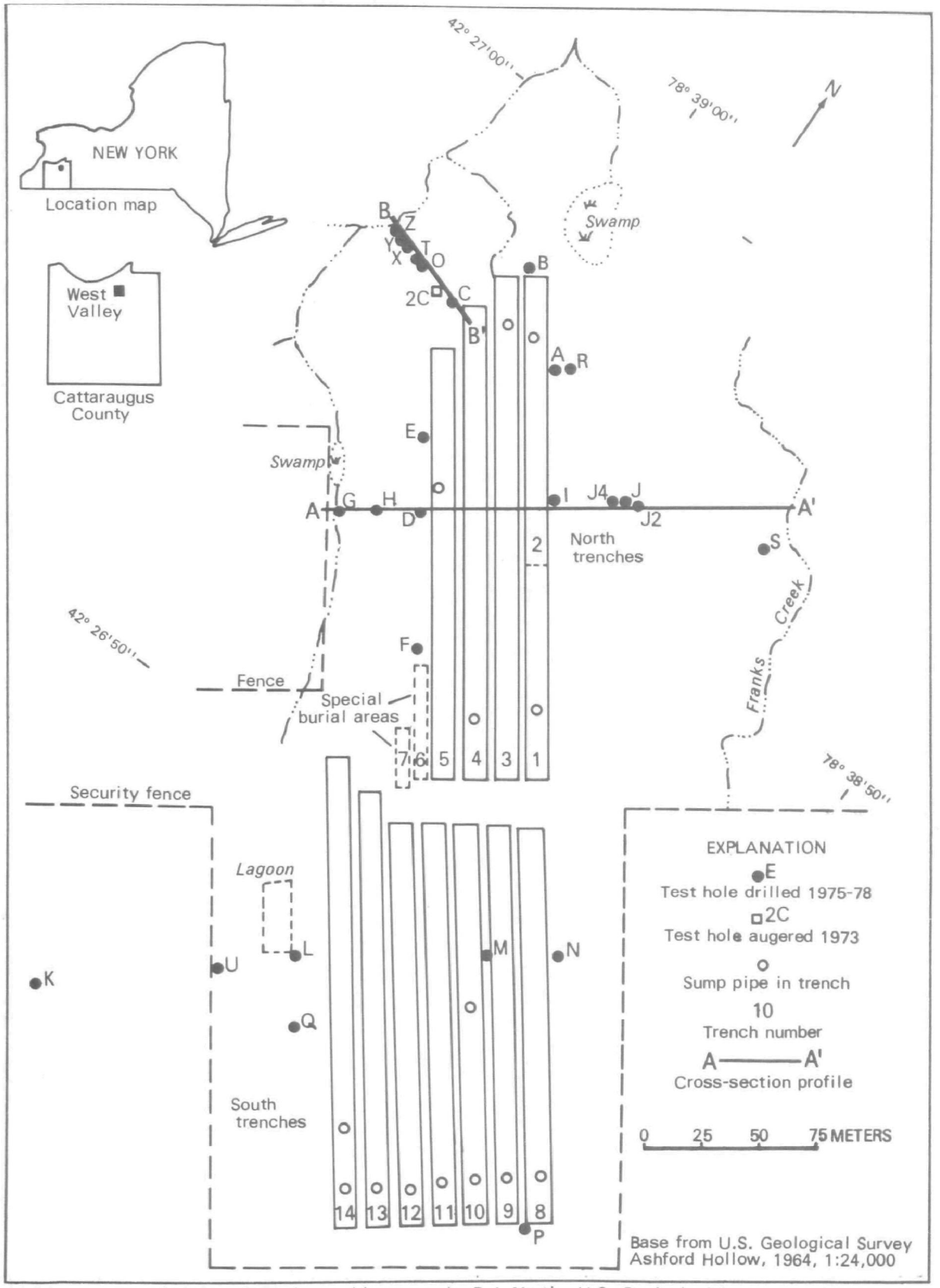
The climate at the center is humid contential with an annual average temperature of 7°C. Temperature extremes range from 38°C during summer to -26°C during winter. Precipitation averages 100 cm/yr without distinctly wet or dry seasons. During winter, precipitation is normally in the form of snow.

Operation of the landfill began in November 1963 and continued until May 1975. The 4-ha (11-acre) landfill contains a series of trenches excavated in silty-clay till of low hydraulic conductivity and containing scattered pods of silt and sand. Radioactive wastes were buried in trenches that are generally 6 m deep, 10 m wide at the surface, and 180 m long (fig. 1). Trenches 6 and 7 were set aside for burial of special material of high specific activity (2).

Purpose and Scope

This study was done as part of a national study by the U.S. Geological Survey to determine the principal factors that control the subsurface movement of radioisotopes at several radioactive-waste landfills. Results of this study have been used in an investigation begun in 1975 by the New York State Geological Survey, as lead agency under contract with the U.S. Environmental Protection Agency, and the U.S. Nuclear Regulatory Agency, to evaluate all processes of radioisotope migration at the site. This report describes results of computer modeling of groundwater flow near the north trenches (fig. 1).

Test holes drilled or augered near the landfill during 1975-78 were designed to provide information about the flow of groundwater as well as the geology. Cores were collected and analyzed to determine the distribution of radioisotopes and to detect possible movement of water away from the burial trenches (3,4). Several laboratory tests were run on selected core samples of the till to determine hydraulic properties. Test holes were assigned a letter, and in the few instances when two or more test holes were drilled in proximity (1 to 3 m of one another), a sequential number followed the letter; for example, test holes I, I2, and I3. (See fig. 1.)



NOTE: Map based on plane-table survey by R.J. Martin, U.S. Geological Survey, 1975-78

Figure 1. Layout of trenches and location of test holes and wells used to monitor water-level trends.

To determine head distribution in three dimensions, each test hole was designed to contain from 1 to 4 piezometers 3 cm in diameter and having a 30-cm-long screen. Each screen was finished in a sand envelope about 45 cm thick. At least 3 m of grout separated piezometers when more than one was finished in a test hole. Two small-diameter tubes (1 cm and 0.5 cm) extended from the screen to land surface. The smallest diameter tubing ended near the bottom of the screen, whereas the larger ended near the top of the screen. The small-diameter tubing was used to minimize the amount of water needed to fill it and thus reduce the lag time between head change in the till and response in the piezometer. The double-tube system was used to obtain periodic water samples.

Piezometers were designated according to test-hole number followed by a number preceded by a hyphen. The numbers designate individual piezometers within a test hole, and piezometers were numbered sequentially from shallow to deep; for example, G-1, G-2, and G-3.

During this investigation, hydrologic studies were limited to the till for the following reasons: (a) the trenches were excavated only in this till; (b) trench cover consisted of reworked till, and (c) radioisotope migration was confined to the till (3,4).

A two-dimensional finite-element model developed by Reeves and Duguid (5) was used to study factors controlling groundwater flow in the till. The objective was to simulate groundwater flow in a cross section perpendicular to the north trenches (nos. 2-5) from test hole G eastward to Franks Creek (fig. 1) because these trenches had had high initial water levels in February 1976 that were lowered by pumping in July 1976. This lowering produced a stress that normally would not have occurred and allowed for better calibration of the model.

Acknowledgments

Mark Reeves (formerly with Oak Ridge National Laboratory) assisted with the initial computer runs and helped adapt the program to the conditions at West Valley. Nuclear Fuels Services, the site operator, provided personnel to monitor radiation levels whenever Survey personnel and their contractors were near or on the burial trenches; also their staff answered many questions about burial procedures and practices. Stephen Mollelo (New York State Geological Survey) and Robert Wozniak (New York State Department of Environmental Conservation) assisted with the data collection.

GEOLOGIC CONDITIONS NEAR LANDFILL

Surficial geologic mapping (6) near the landfill defined the nature and extent of the till in which the burial trenches are excavated. The till, composed predominantly of silt and clay, is a valley facies that

is widely distributed in the Cattaraugus Creek basin. It is found below the level of saddles in the drainage divide to the south and must have been deposited by an ice sheet partly suspended in ponded water.

The till is commonly covered by thin gravel deposits (6) that, at the landfill, are largely absent. The till extends to about 30 m below land surface near the trenches and overlies a bedded lacustrine unit 10 to 20 m thick consisting of fine sand and silt and locally capped by gravel. The upper part of the lacustrine unit is unsaturated (fig. 2).

Bedrock is as much as 150 m below land surface near the trenches. Although the geology and hydrology of the thick glacial deposits beneath the lacustrine unit are largely unknown, the lacustrine unit probably provides an avenue for slow lateral flow to points of discharge in the bluff along Buttermilk Creek, 550 m northeast of the landfill (3).

Fourteen till samples from test holes near the landfill were analyzed for particle size. On the average, the samples contained 50 percent clay, 27 percent silt, 10 percent sand, and 13 percent gravel; LaFleur (6) reported that 10 to 20 percent pebbles and cobbles is characteristic at most exposures. Typically the unsorted till interfingers with a similar till having a pebble content of less than 5 percent and a matrix containing tiny blebs and torn, deformed wisps of quartz silt; this latter till constitutes between 20 and 25 percent of the till thickness (6). The unsorted till also includes thin layers of silt, sand, and rarely coarser sand, which together constitute about 7 percent of the core footage logged (3). Both subunits were encountered in all test holes (fig. 2). However, stratified materials penetrated by nearby test holes commonly differ appreciably in altitude and(or) lithology, and even where altitude and lithology are similar, the steep dips indicated by many of the cores and exposures seem to negate the possibility of a continuous subhorizontal layer that could indicate a widespread inplace glaciofluvial deposit.

Distribution of Fractures in Till

A network of intersecting horizontal and vertical fractures characterizes the oxidized upper 2 m of the till near the landfill. Fractures and root tubes whose surfaces are bordered by firm oxidized till were recognizable to depths of 3 m to 4.5 m in cores from several test holes next to the landfill (3). Some vertical fractures extend downward into the unweathered till. Dana and others (7) noted that the number of fractures and their degree of openness decreased with depth in excavations near the landfill. Both manganese and calcite deposits have been observed along several fractures in excavations and also in cores from test holes next to the landfill. Results from a laboratory study (8) suggests that the theoretical limit to which a fracture could penetrate in the till is about 15 m.

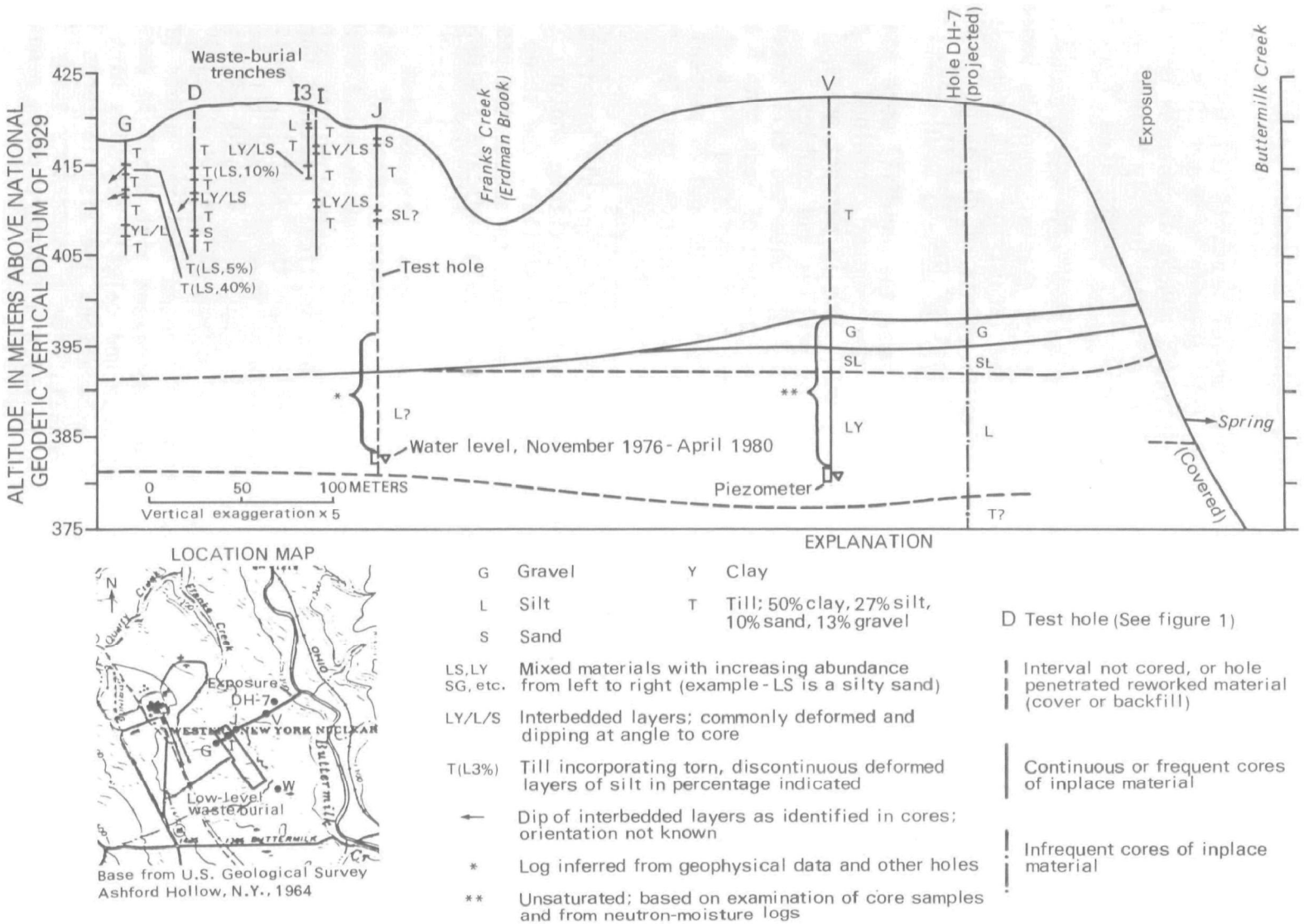


Figure 2. Generalized cross section from test hole G to Buttermilk Creek. Spring may be perched water of local origin; flow is probably less than 1 liter per minute. (Modified from Prudic and Randall, 1979.)

GROUNDWATER FLOW NEAR THE NORTH TRENCHES

Much of the precipitation on the landfill either runs off to nearby streams and gullies or returns to the atmosphere by evapotranspiration (3). The small amount that infiltrates below the roots of plants moves generally downward, even beneath small valleys bordering the site, as indicated by the distribution of hydraulic head along a section perpendicular to the north burial trenches in February 1976 (fig. 3). At that time, most of the north trenches were nearly filled with water (3) that was generally moving outward and downward from the trenches. A small flow component toward trench 5 may be inferred from the hydraulic head near land surface within 10 m west of the trench (fig. 3).

Pressure head within the till ranged from near zero to more than 5 m. Low-pressure heads generally occurred beneath steep and(or) smooth slopes or where the upper layers of soil were scraped to allow for rapid and complete runoff. Pressure heads in the till were generally greater where water had accumulated above the till, as in the trenches, in natural depressions in land surface (as near holes J and G in fig. 1), and in remnants of late-glacial fluvial gravel atop the till (3).

Response of Water Levels in Piezometers to Pumpout of Water from Trenches 2-5

Water was pumped from trenches 3, 4, and 5 on several dates between July and November 1976 to lower the water levels and was pumped again between August and November 1977, including trench 2. The piezometers next to trenches 5 and 2 responded to the pumpout (figs. 4 and 5), but those farther away showed no response (fig. 6).

The decline of water levels in piezometers near trench 5 was most rapid in those finished in undisturbed material near the reported altitude of the trench floor (D-1, E-2, and F-2) or in a sandy backfill next to the trench (E-1) (3).

The sudden water-level increases in piezometers D-2 and F-3 (fig. 4) in May and June 1976 were caused by attempts to sample the piezometers, whereby nitrogen was injected at pressures as high as 4.2 kg/cm^2 down the larger of two tubes that extended to the piezometer screen* which forced water up the smaller tube to the surface. Apparently pressures were large enough to deform the till and spread it away from the column of hardened cement grout above the piezometer, in effect increasing the length of piezometer. Because total head in the till declines with depth, the water level rose when water from shallower depth entered the piezometer. The subsequent decline in water level reflects partial resealing of till against the grout column as well as a response to trench pumpout.

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* Other piezometers were sampled by suction lift in combination with gas pressures less than 0.5 kg/cm^2.

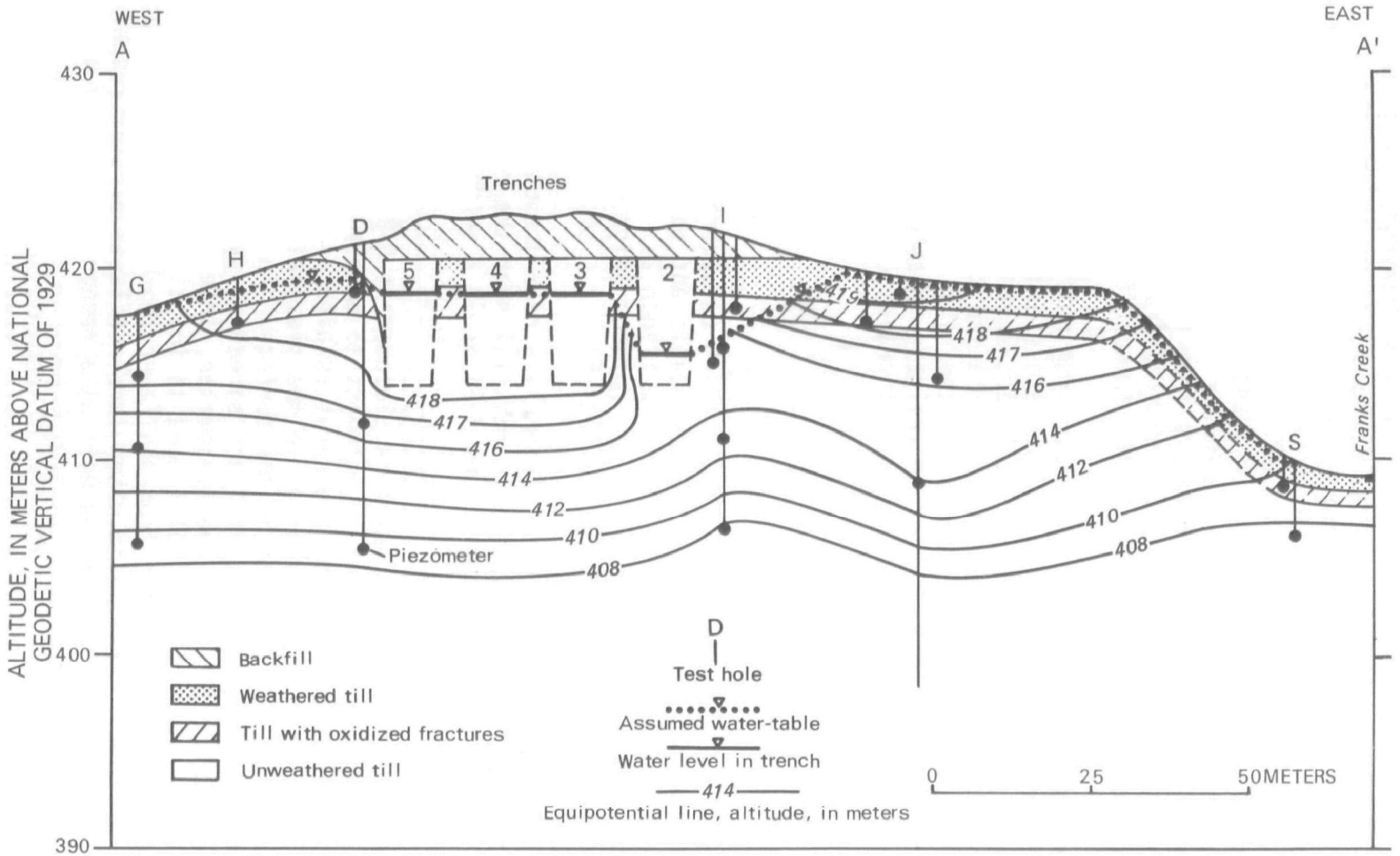

Figure 3. Cross section A-A' through north trenches showing head distribution, February 1976. (Location of section is indicated in fig. 1.)

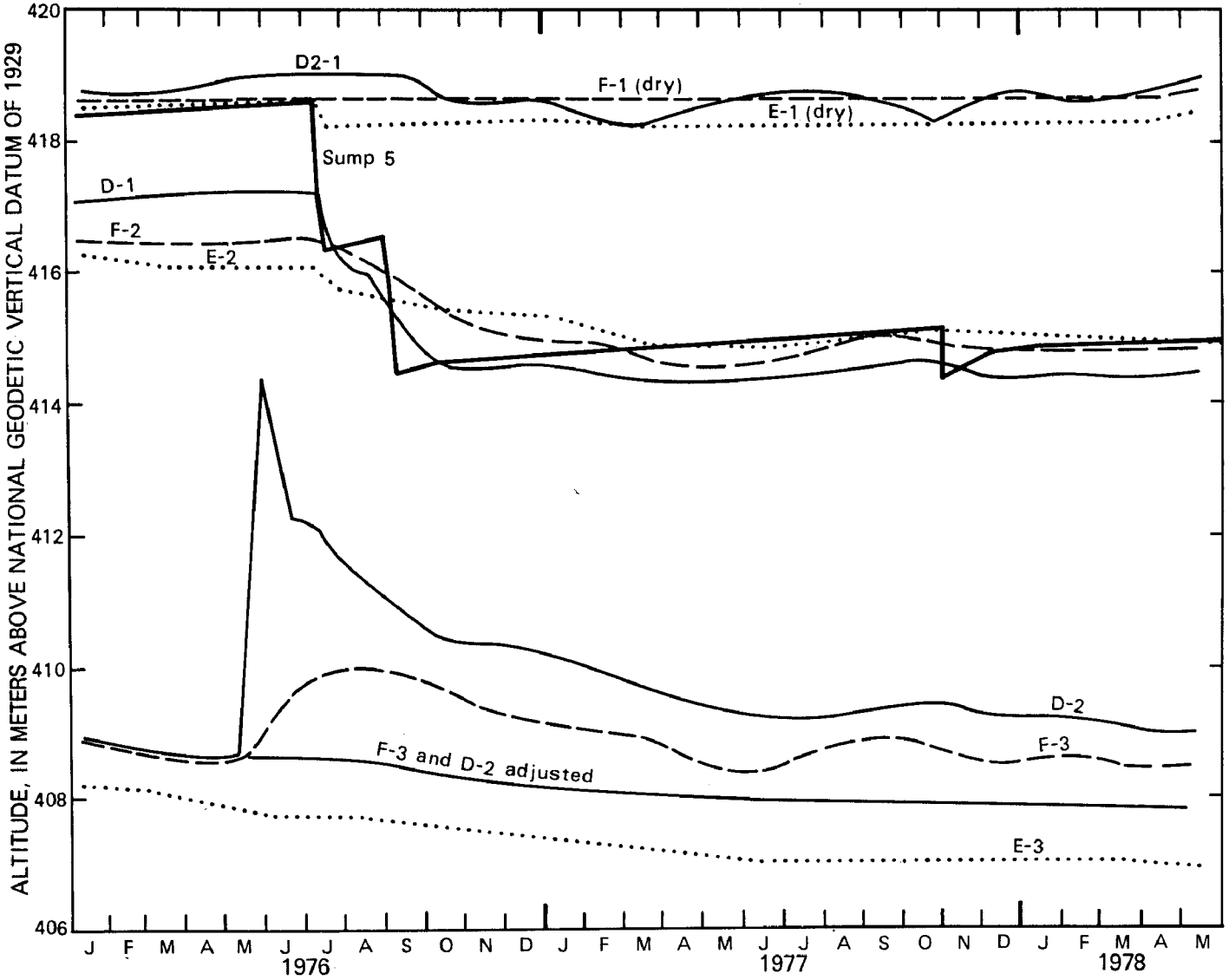

Figure 4. Water-level trends in piezometers finished next to trench 5. (Letter and number identifies piezometer, sump refers to well in trench.)

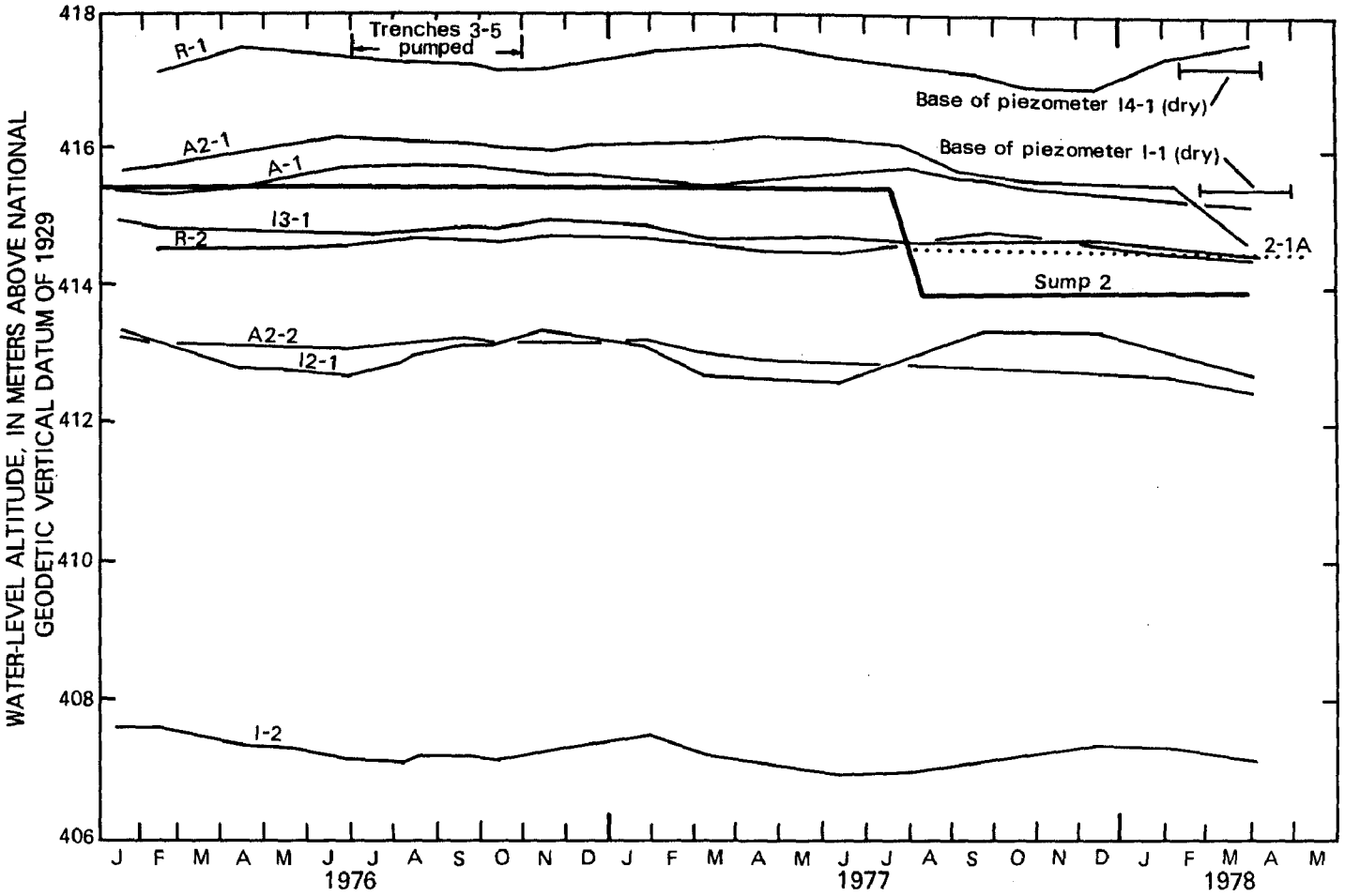

Figure 5. Water-level trends in piezometers finished next to trench 2. (Letter and number identifies piezometer, sump refers to well in trench.)

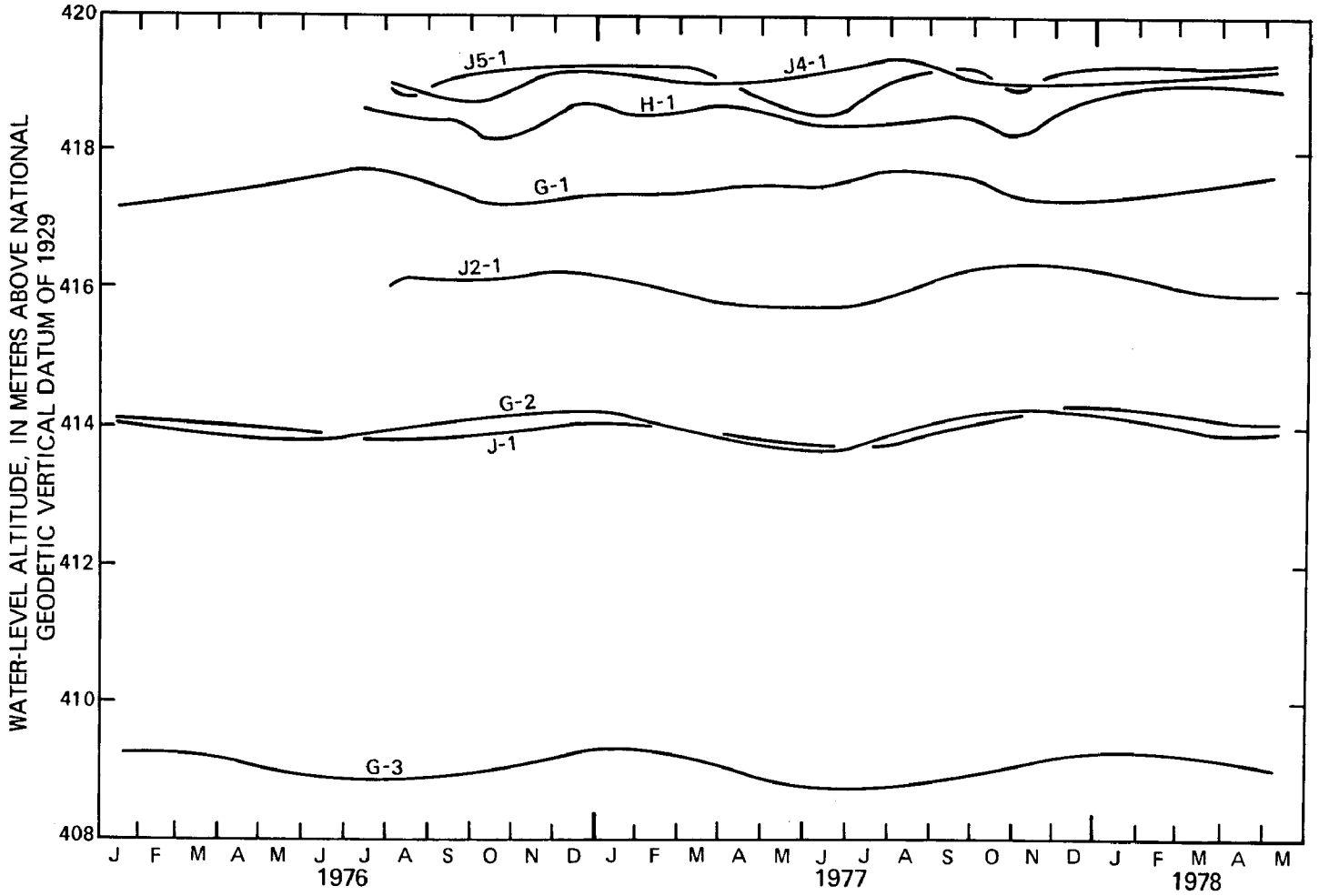

Figure 6. Water-level trends in piezometers finished distant from trenches 2 through 5. (Letter and number identifies piezometers.)

Although the two effects cannot be separately measured, for purposes of model calibration, the water-level trends in piezometers D-2 and F-3 caused by the pumpouts were estimated from measurements in E-3, which was finished at similar depth along the west side of trench 5.

The decline in water level in piezometers next to trench 2 was less pronounced than that next to trench 5. Because water level in trench 2 was lower than in trench 5, the decrease in water level was less. Of the piezometers finished next to trench 2, A2-1, finished in a lens of layered silt and fine sand that dips from piezometer R-1 toward trench 2, responded most rapidly (fig. 5). Piezometers in test hole R, 6 m east of those in test holes A and A2 (fig. 1), did not show a decline beyond the normal yearly fluctuations (fig. 4).

Test holes I, I2, I3, and I4 are near the south end of trench 2, about 70 m from the sump from which water was pumped out of trench 2 (fig. 1). Well 2-1A, driven into trench 2 in June 1976 near test hole I, had nearly the same water level as the sump until the sump water was lowered below an altitude of 414.5 m (fig. 4); however, continued pumping from the sump did not cause a decrease in well 2-1A. After the pumpout of trench 2, the difference between water-level trends in piezometers at the north end and those at the south end probably reflects differences in water level within trench 2 itself.

Hydraulic Properties of Saturated and Unsaturated Till

Hydraulic conductivity of the saturated unfractured till was obtained from both field and laboratory studies. Field tests were done by withdrawing 200 to 500 ml of water out of piezometers finished at depths from 5 to 16 m, then measuring the water-level rise in the piezometers until they had stabilized.

Two methods were used to analyze the data. The first assumed horizontal flow to the piezometer (9); the second assumed spherical flow (10). Average hydraulic conductivity calculated from 12 tests was 6×10^{-8} cm/s by the first method and 2×10^{-8} cm/s by the second. Hydraulic conductivity measured in laboratory tests at confining pressures on seven core samples from depths of 5 to 16 m produced an average vertical hydraulic conductivity of 2×10^{-8} cm/s, which compares well with values obtained from field tests that assumed spherical flow. Fickies and others (8) reported anistropy with 40 times greater horizontal than vertical conductivity in two core samples, although laboratory tests of nine core samples suggest little or no anistropy. Analyses of thin sections of 18 till samples do not suggest preferential horizontal layering of the clay grains within the till.

Consolidation tests were run on four samples to determine the effects of increased confining pressures on hydraulic conductivity. In general, the vertical hydraulic conductivity decreased by about 40 percent as confining pressures increased from near atmospheric to 7 kg/cm^2 (equivalent to pressure at a depth of 30 m), which suggests that

increased overburden pressures may reduce hydraulic conductivity of the till (fig. 7). However, much of this decrease occurred at confining pressures between near atmospheric and 1 kg/cm^2. A decrease of less than 10 percent was observed between pressures of 1 to 3.5 kg/cm^2 (equivalent to pressure at a depth of 5 to 16 m), and at pressures from 3.5 to 7 kg/cm^2, the decrease averaged 13 percent.

Field tests of seven piezometers finished in small lenses of silt and sand yielded an average hydraulic conductivity of 2 x 10^{-6} cm/s; their range of values (7 x 10^{-8} to 6 x 10^{-6} cm/s) was considerably greater than the range for till. (Weighted average hydraulic conductivity of the till and sorted materials was calculated to be 8 x 10^{-8} cm/s.)

Porosity of the till was determined by measuring dry unit weight and specific gravity of 28 core samples as described by Morris and Johnson (11). Average porosity was 32.4 percent with a standard deviation of 4.7 percent.

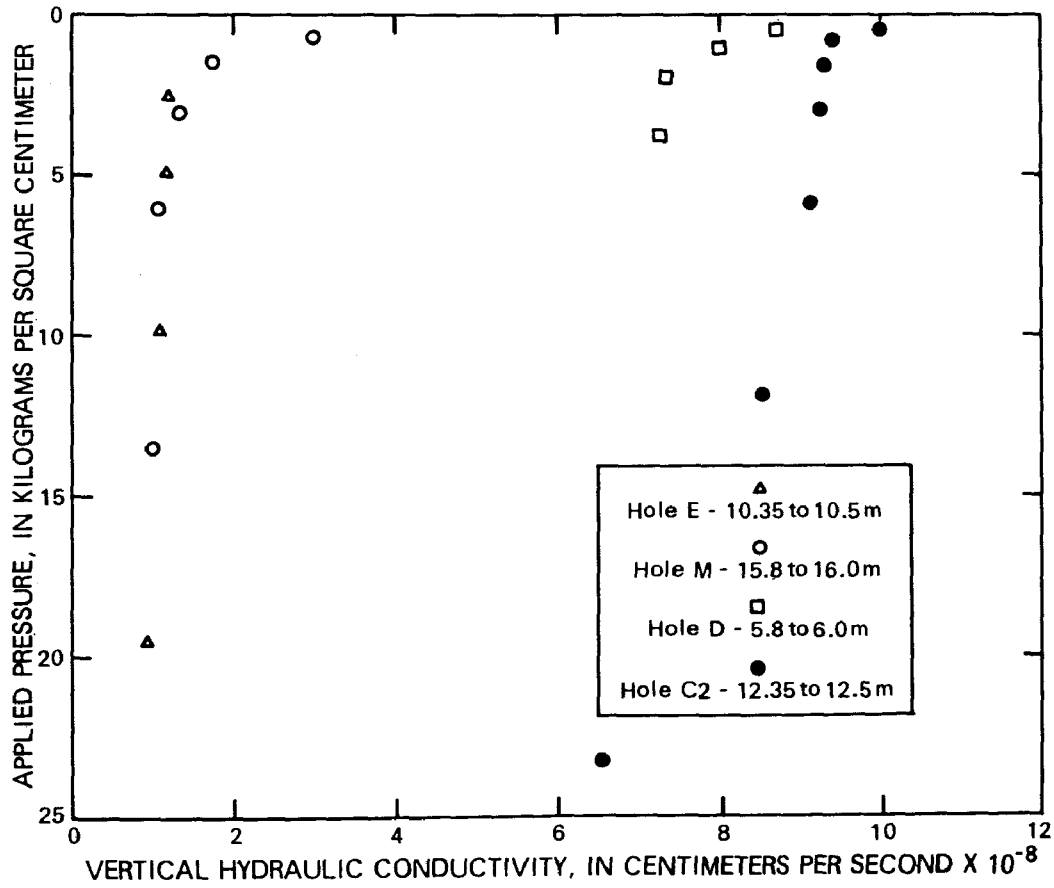

Figure 7. Relationship of hydraulic conductivity to confining pressures as determined from consolidation tests.

Because the model simulates unsaturated as well as saturated conditions, functions relating volumetric moisture content and hydraulic conductivity to soil-moisture tension were needed. Both functions were assumed to be nonhysteretic and were calculated from pore-size-distribution curves derived from mercury porosimeter tests (12) of seven core samples of till. The curves relating soil-moisture content to soil-moisture tension were calculated on the assumption that the capillary pressure of mercury is 5.2 times that of water in air (12). Curves relating hydraulic conductivity to soil-moisture tension were calculated from the soil-moisture curves with an equation by Millington and Quirk (13); both curves used in the model are depicted in figure 8. Saturated hydraulic-conductivity values calculated from the soil-moisture tension curve and an equation by Marshall (14) averaged 6×10^{-8} cm/s, which is reasonably close to measured values.

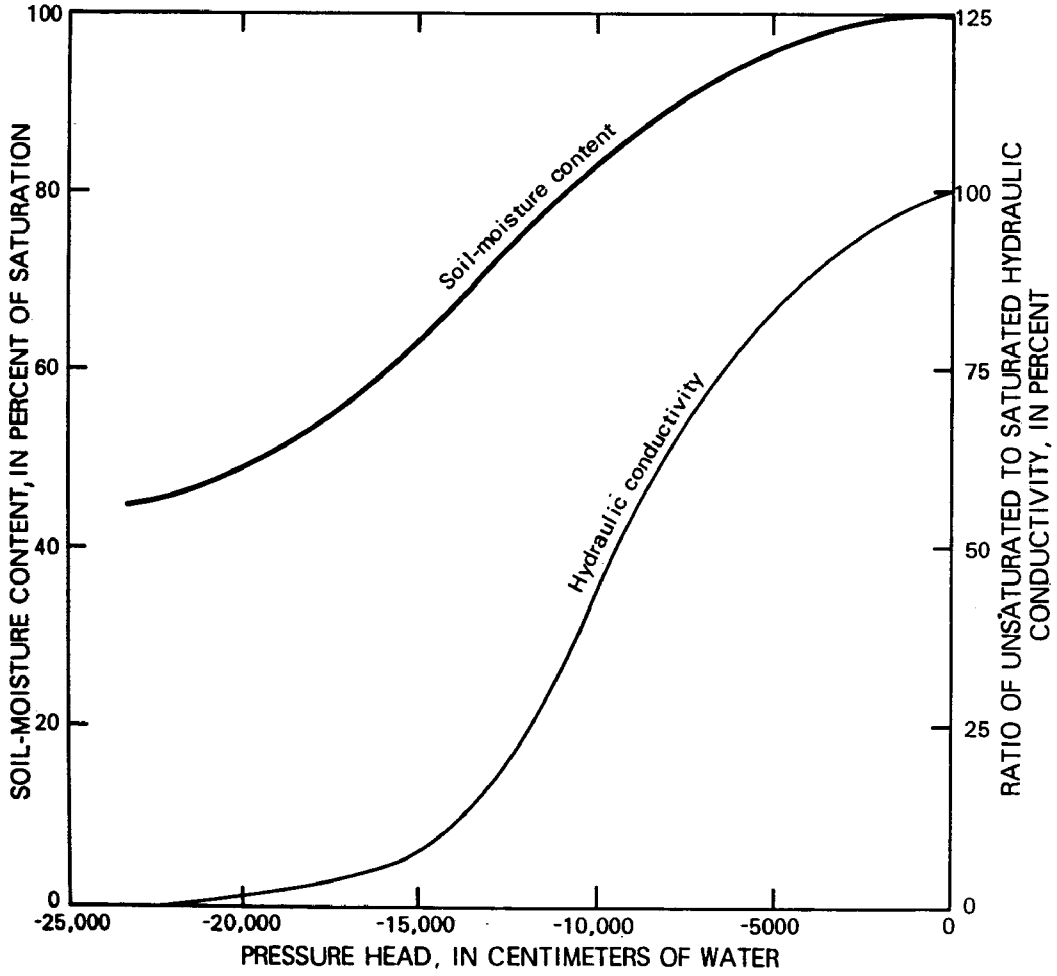

Figure 8. Relationship of hydraulic conductivity and volumetric soil-moisture content to soil-moisture tension, as calculated from seven mercury porosimeter tests of the till.

It was not considered necessary to then relate the computed curves to measured values, as is often required, because the till was nearly saturated, even with soil-moisture tensions exceeding 1,000 cm.

To simulate transient conditions of groundwater flow at the burial site, data on storage within the geologic materials are needed. The storage equation used in the model uses the modified terms of compressibility for water and the solid matrix (5); the modified term of compressibility of water was obtained by multiplying the compressibility of water at 10°C (15) by the density of water and by gravity. The value used in model simulations was 4.3×10^{-8} cm^{-1}.

Specific storage, which is the sum of the modified terms of compressibility of the water and the till, was calculated from the four consolidation tests described previously. The specific storage value of the till, which averaged 8×10^{-6} cm^{-1}, consistently decreased with increasing confining pressures, similar to the hydraulic-conductivity values of the till. Specific-storage values ranged from 16×10^{-6} cm^{-1} at a depth of 5.8 m to 2×10^{-6} cm^{-1} at a depth of 16 m. These values are essentially the modified term of compressibility of the matrix because the value of water compressibility is much lower.

The specific storage values obtained from the consolidation tests are in the lower range of values typical of a medium-hard clay as presented by Domenico and Mifflin (16) and an order of magnitude less than intergranular values presented by Grisak and Cherry (17) for a clay-rich till in Manitoba, Canada.

COMPUTER MODELING OF GROUND-WATER FLOW PERPENDICULAR TO NORTH TRENCHES

The groundwater flow model developed by Reeves and Duguid (5) was chosen for the study at West Valley because it is capable of simulating (a) saturated and unsaturated flow with a moving water table, in cross sections, (b) groundwater outflow to land surface, and (c) temporal variation in inflow from precipitation. Other reasons include (d) no restrictions on the number of units with varying hydraulic properties; (e) no maximum difference between hydraulic-conductivity values of model units; (f) use of constant infiltration rate from land surface during steady-state simulations; and (g) availability of a solute model that was developed and coupled to the flow model (18).

Reeves and Duguid (5) stated that the equations representing flow in saturated and unsaturated porous media consist of equations of (a) continuity of the water; (b) continuity of the matrix; (c) motion of the water; (d) consolidation of the matrix, and (e) compressibility of the water and combined these equations into one:

$$\left(\frac{\theta}{n}\alpha' + \theta B' + \frac{d\theta}{dh}\right)\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[\vec{K}\left(\frac{\partial h}{\partial x}\right)\right] + \frac{\partial}{\partial z}\left[\vec{K}\left(\frac{\partial h}{\partial z} + 1\right)\right] \qquad (1)$$

Where θ = volumetric moisture content, dimensionless ratio;

η = porosity, dimensionless ratio;

β' = modified coefficient of compressibility of the water, L^{-1};

α' = modified coefficient of compressibility of medium, L^{-1};

$\frac{d\theta}{dh}$ = change in moisture content with respect to pressure head, L^{-1};

$\frac{\partial h}{\partial t}$ = change in pressure head with respect to time, LT^{-1};

$\vec{K}$ = hydraulic conductivity tensor, LT^{-1};

h = pressure head, L;

z = vertical distance, L;

x = horizontal distance, L.

This equation reduces to Richard's equation (19) for unsaturated flow and reduces to the elastic storage equation for saturated flow (5). Because the model solves for total head, both equations are automatically satisfied.

The hydraulic-conductivity tensor is dependent on pressure head, as shown in the following equation:

$$\vec{K} = \vec{K}_s \cdot K_r(h) \qquad (2)$$

Where K = hydraulic-conductivity tensor, LT^{-1};

$\vec{K}_s$ = saturated-hydraulic conductivity tensor, LT^{-1};

$K_r(h)$ = relative hydraulic conductivity as function of pressure head, dimensionless.

Steady-State Simulations

A finite-element grid was developed to represent the cross section A-A' from hole G east to Franks Creek (fig. 1). The following conditions were established for steady-state simulation of flow in February 1976 and February 1978:

(a) No-flow boundaries were assigned to both sides of the section because hydraulic gradient is predominantly vertical.

(b) The silt was modeled at a pressure head of zero at the base of the till because the silt underlying the till is generally unsaturated.

(c) Infiltration from precipitation was at a steady rate sufficient to saturate the till to land surface; however, the rate was decreased in some model runs to create local unsaturated conditions.

(d) A horizontal hydraulic conductivity of 8×10^{-8} cm/s was assigned to the unweathered till unit; this is a weighted average hydraulic conductivity of the till and the sorted material.

(e) Constant head within the trenches was made equal to observed head in February 1976 or February 1978. (This assumption of constant head in the trenches is reasonable for periods of 2 to 3 months because the water level in these trenches did not generally change more than 5 cm in a month.)

Several steady-state simulations were run to evaluate the relative significance of anisotropy, variations in hydraulic conductivity caused by fracturing and increased confining pressures within the till, and infiltration from precipitation. Simulations became progressively more complicated, starting with a single isotropic unit but eventually considering as many as five units with varying degrees of anisotropy. The mean absolute departure of simulated heads from heads observed at 17 piezometers in the plane of the section was calculated for each model run as a general index of degree of fit; the results are given in table 1.

Simulations that incorporated a single isotropic unit yielded the same pressure heads regardless of hydraulic conductivity (table 1, case 1); however, changes in computed inflow and outflow rates were directly proportional to any change in hydraulic conductivity. Simulations that incorporated a single anisotropic unit produced better fits (decreased the mean absolute departure), and best results were obtained when horizontal hydraulic conductivity was 100 times the vertical value (table 1, case 2). Simulating several shallow isotropic layer(s) at a hydraulic conductivity greater than 8×10^{-8} cm/s to represent the abundantly fractured weathered till and the fractured unweathered till also produced better fits than a single isotropic unit, and best results were obtained when the hydraulic conductivity was between 10 and 100 times higher in the weathered till than in the unweathered till (table 1, cases 3 and 7). Simulating anisotropy of the layered units reduced the mean absolute departures (table 1, cases 4, 5, 6, and 8).

Most simulations incorporated an infiltration rate large enough to saturate the till to land surface, but infiltration rates in a few simulations were reduced enough to cause the uppermost nodes of the model to become unsaturated. When anisotropy was included, the result was a slight lowering of heads in most nodes in the section. In isotropic simulations, large changes in heads occurred in the nodes beneath points where infiltration was the only source of water. For example, reducing infiltration rate near model holes D and I did not greatly affect heads

Table 1. Differences between heads observed in February 1976 and simulated heads for assumed conditions.

Case	Conditions	Mean absolute departure from observed heads of February 1976 (centimeters)
1	one isotropic unit	
	(a) $Kx = Kz = 3.0 \times 10^{-8}$ cm/s	201
	(b) $Kx = Kz = 3.0 \times 10^{-7}$ cm/s	201
2	one unit with anisotropy	
	(a) $Kz = 0.1\ Kx$	161
	(b) $Kz = 0.01\ Kx$	114
	(c) $Kz = 0.001\ Kx$	116
3	two isotropic units (weathered and unweathered till)	
	(a) K (weathered) = 10 K (unweathered)	123
	(b) K (weathered) = 100 K (unweathered)	127
4	two anisotropic units (weathered and unweathered till)	
	Kx (weathered) = 10 Kx (unweathered)	
	(a) Kz = 0.1 Kx in each unit	93
	(b) Kz = 0.01 Kx in each unit	74
5	two anisotropic units (weathered and unweathered till)	
	Kx (weathered) = 100 Kx (unweathered)	
	(a) Kz = 0.1 Kx in each unit	90
	(b) Kz = 0.1 Kx (weathered)	
	Kz = Kx (unweathered)	109
	(c) Kz = 0.01 Kx (weathered)	
	Kz = 0.01 Kx (unweathered)	92
6	two anisotropic units (weathered and unweathered till)	
	Kx (weathered) = 10 Kx (unweathered)	
	Kz = 0.01 Kx in each unit	
	(a) simulated sand and silt lenses near D, I, and J	65
	(b) as above plus increased heads at base of model near G	60

Table 1. Differences between heads observed in February 1976 and simulated heads for assumed conditions. (Continued)

Case	Conditions	Mean absolute departure from observed heads of February 1976 (centimeters)
7	Three isotropic units (weathered, unweathered with fractures and unweathered till)	
	(a) K (weathered) = 10 K (unweathered) K (unweathered w/fractures) = 5 K (unweathered)	116
	(b) K (weathered) = 100 K (unweathered) K (unweathered w/fractures) = 10 K (unweathered)	121
8	Three anisotropic units (weathered, unweathered with fractures and unweathered till) with Kx the same as noted in case 7(a) above	
	(a) Kz = 0.1 Kx in each unit	96
	(b) Kz = 0.01 Kx in each unit	93
	(c) Kz = 0.01 Kx in each unit plus simulated sand and silt lenses near D, I, and J; increased head at base of model near G, and lower infiltration near holes D and I	57
	(d) same as 8(c) except Kz = 0.1 Kx for each unit	53
9	Four isotropic units (weathered, unweathered with fractures, and 2 unweathered till units to compensate for overburden pressures) K (weathered) = 10 K (unweathered) K (unweathered w/fractures) = 5 K (unweathered)	
	(a) K (lowest unweathered unit) = 0.5 K (unweathered)	120
	(b) K (lowest unweathered unit) = 0.7 K (unweathered)	104
	(c) K (lowest unweathered unit) = 0.85 K (unweathered)	107
	(d) K (lowest unweathered unit) = 0.7 K (unweathered) plus simulated sand and silt lenses near D, I and J; and reduced infiltration near D and I	31
	(e) as above, but K (lowest unweathered unit) = 0.85 K (unweathered) except beneath hole G where K (lowest unweathered unit) = 0.7 K (unweathered)	21

in nodes below the bottom of the trenches, whereas it did near holes H and J. Infiltration rates near swampy areas were adjusted to saturate the till barely to land surface. The final infiltration rate used in the computer simulations was about 3.8 cm/yr near swampy areas, whereas the model infiltration rate near hole I was 1.5 cm/yr.

In all model runs, simulated heads in the deepest piezometer at hole G were lower than observed heads. This would be expected if the lacustrine silt or sand beneath the till south and east of the trenches became thinner to the west, pinching out near hole G, or that the unit became finer toward the west. Because this unit seems to be unsaturated beneath the trenches, such a thinning out or fining of the sediments would indicate saturated conditions near hole G at the altitude of 391 m. In this case the model boundary below hole G would be represented by pressure heads greater than zero. Although this hypothesis is unproved, it seems plausible from records of test holes in the area. Alternatively, the till at depth beneath hole G could have a slightly lower hydraulic conductivity. Pressure head in the piezometers in hole G was reasonably simulated assuming isotropic conditions and assuming hydraulic conductivity of the till below 400 m altitude beneath hole G to be 30 percent less than that of the unweathered till. Although neither assumption has been proved, the latter seems more reasonable than assuming slightly positive heads at the base of the till near hole G.

The best simulations with anisotropy included three units (the weathered zone, the unweathered till with fractures, and the unweathered till), and also included localized silt and sand lenses near piezometers D-1, J-1, and I2-1. In these tests the weathered till unit had a horizontal hydraulic conductivity 10 times higher than the unweathered till with oxidized fractures, whereas the localized silt and sand units had values 5 times higher than the unweathered till. The horizontal hydraulic conductivity in all three till units was 10 times higher than the vertical; the localized silts and sand lenses were assumed to be isotropic. The mean absolute departure in this run was 53 cm (table 1, case 8d).

The best simulations assumed four isotropic till units with the horizontal hydraulic conductivities described above, plus an additional unit below the 400-m altitude beneath the trenches and 396 m beneath Franks Creek. The hydraulic conductivity of this unit was 6.9×10^{-8} cm/s, or 15 percent less than that of the unweathered till except below hole G, where the value was 5.6×10^{-8} cm/s. The purpose of this lower unit was to represent the reduction in hydraulic conductivity with depth, either from greater overburden pressure or the lower percentage of disturbed silt and sand layers below 400 m, as suggested by some of the test borings. A four-unit model was also hypothesized by field observations in test trenches dug near the burial ground (7).

The above simulations included localized silt and sand lenses near piezometers D-1, J-1, and I2-1. The mean absolute departure in this run was 21 cm. Figure 9 depicts the nodes, boundary conditions, and the relative hydraulic-conductivitiy values used in the best-fit model simulations.

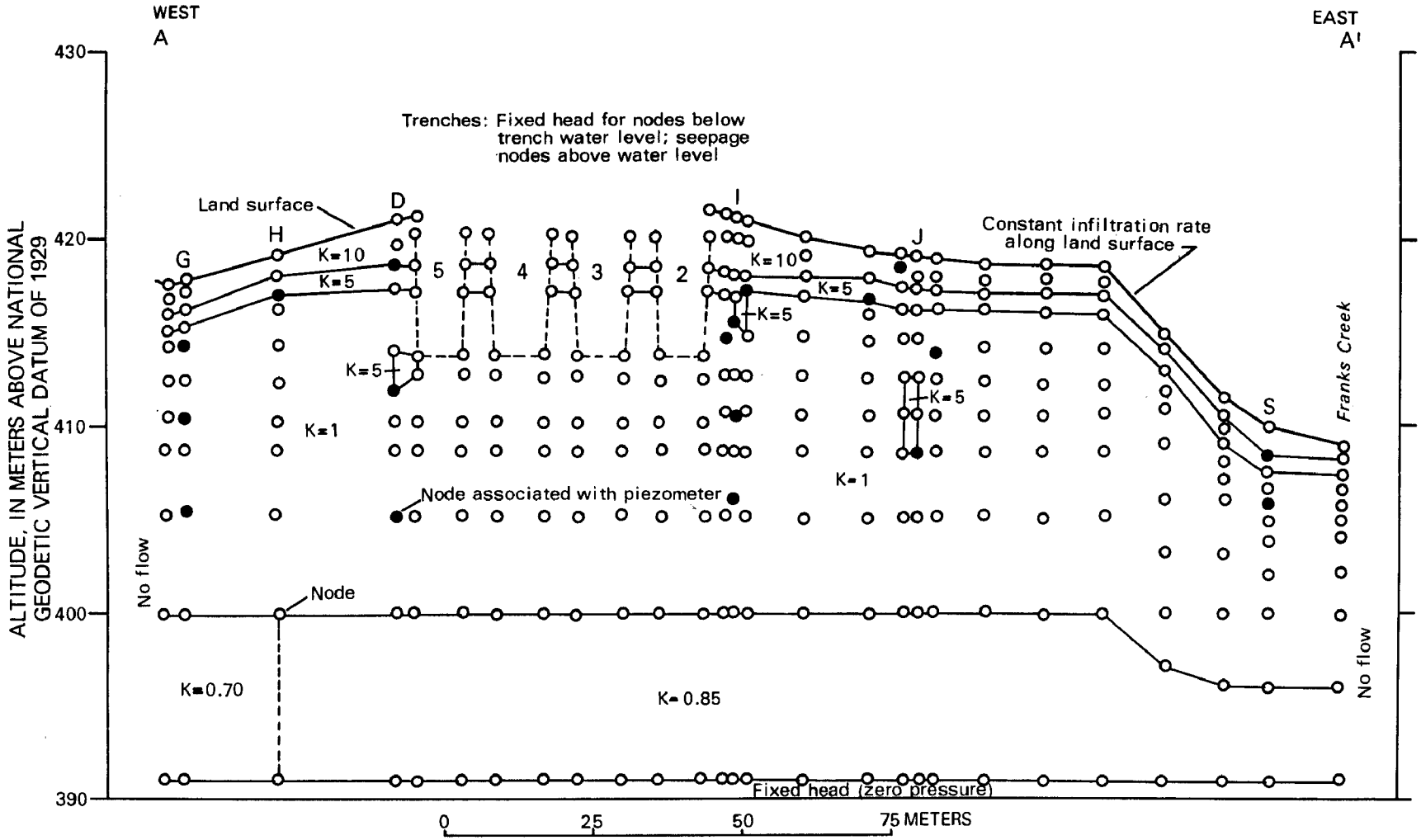

Figure 9. Cross section A-A' through north trenches showing arrangement of nodes, boundary conditions, and relative hydraulic conductivities used to best-fit model simulation.

Table 2 compares simulated values for best computer simulations with observed values for both anisotropic and isotropic conditions for both February 1976 and February 1978. The isotropic four-layer simulations produced smaller average departures than the anisotropic three-layer simulations and also were qualitatively more reasonable in at least two respects: (a) they yielded negative heads at piezometers I-1 and I4-1, which were dry on both dates, whereas the best anisotropic simulations yielded positive heads, and (b) they also yielded about the same heads on both dates in the piezometers at hole G, in agreement with observed conditions, whereas the best anisotropic simulations yielded significantly lower heads at hole G in February 1978 in response to the lower water level simulated in the trenches.

The distribution of heads within the till during February 1976 and 1978, based on the best steady-state computer simulations, are shown in figures 10 and 11. From the simulation of February 1976, water moving from trench 5 would flow outward only 2 to 3 m before it would move downward; the same pattern is indicated east of trench 2. In February 1978, the outward movement of water was less than 2 cm/yr. Average computed vertical flow rate beneath the trenches was 3 cm/yr in February 1976 and less than 2 cm/yr in February 1978. These model simulations indicated a groundwater discharge to land surface west of hole G and on the lowest part of the slope near the east side of the model; then model discharges averaged 100 cm^3/d (0.05 gallons per day) per m^2 of surface but occurred only over small areas and were derived largely from flow through the weathered till. These rates could not be verified in the field because the streams bordering the landfill are small and during summer are dry much of the time. In addition, streamflow could not be measured to the accuracy required to determine such small seepage rates. However, near the computed areas of discharge are marshy areas that could be the result of shallow groundwater seepage.

Although the steady-state model simulations reproduced observed heads in the till from hydraulic properties obtained from field and laboratory measurements, the simulations could not independently define the hydraulic conductivity of the till because the same heads could be simulated by changing all values of hydraulic conductivity and infiltration by a proportionate amount.

Transient-State Simulations

Transient conditions were simulated in an attempt to reproduce the observed drawdowns in piezometers finished in the till after the pumpout of water from trenches 3-5 in the summer of 1976. Initial calibration of the flow model was obtained by simulating the drawdown in piezometer D-1 after the pumpout of trench 5 from July 7-17, 1976.

Figure 12 compares observed water levels in piezometer D-1 with simulated values resulting from different specific-storage values. The best fit was obtained from a specific-storage value of 16×10^{-6} cm^{-1}.

Table 2. Heads observed in February 1976 and February 1978 compared with results of best-fitting computer simulations for isotropic and anisotropic conditions

[All values are in centimeters]

Piezometers	Observed heads	Calculated heads from best computer simulation with anisotropy (table 1: case 8, part d)	Absolute departure from observed heads	Calculated heads from best computer simulation with isotropic conditions (table 1: case 9, part e)	Absolute departure from observed heads
February 1976					
G-3	382.	254.	128.	359.	23.
G-2	374.	276.	98.	330.	44.
G-1	320.	291.	29.	307.	13.
H-1	178.	187.	9.	187.	9.
D2-1	47.	46.	1.	47.	0.
D-2	348.	308.	40.	359.	11.
D-1	562.	629.	67	560.	2.
I3-1	68.	142.	74.	89.	21.
I-2	169.	218.	49.	173.	4.
I2-1	248.	220.	28.	180.	68.
I-1	dry	91.	>91.	-79.	-.
I4-1	dry	144.	>144.	-96.	-.
J4-1	214.	202.	12.	219.	5.
J5-1	84.	45.	39.	46.	38.
J-1	545.	537.	8.	524.	13.
J2-1	235.	166.	69.	288.	57.
S1-6	260.	221.	39.	262.	4.
S2-1	178.	140.	38.	152.	25.
February 1978					
G-3	387.	179.	208.	360.	27.
G-2	386.	221.	165.	329.	57.
G-1	327.	277.	50.	304.	23.
H-1	225.	177.	48.	188.	37.
D2-1	47.	26.	21.	15.	32.
D-2	246.	172.	74.	220.	26.
D-1	285.	322.	37.	268.	17.
I3-1	39.	94.	55.	73.	34.
I-2	137.	155.	18.	152.	15.
I2-1	224.	152.	72.	158.	66.
I-1	dry	67.	>67.	-22.	-
I4-1	dry	32.	>32.	-154.	-
J4-1	221.	200.	21.	220.	1.
J5-1	75.	45.	30.	48.	27.
J-1	561.	526.	35.	520.	41.
J2-1	260.	158.	102.	286.	26.
S1-1	261.	221.	45.	262.	1.
S2-1	181.	138.	43.	152.	29.
Mean absolute departure			1976=53. 1978=62.		1976=21. 1978=29.
Standard deviation			1976=41. 1978=51.		1976=27. 1978=17.

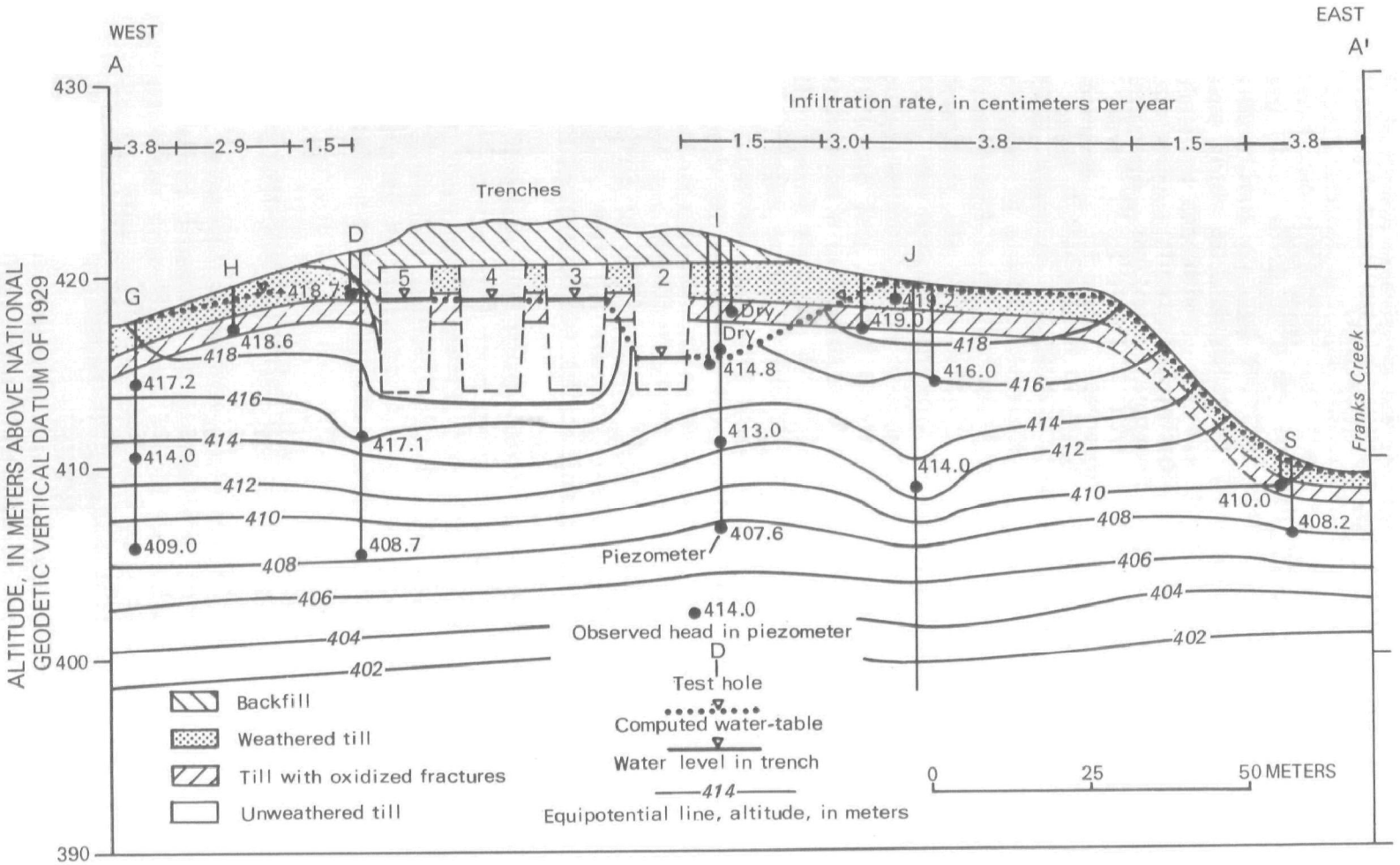

Figure 10. Cross section A-A' through north trenches showing computer-simulated distribution of head in February 1976.

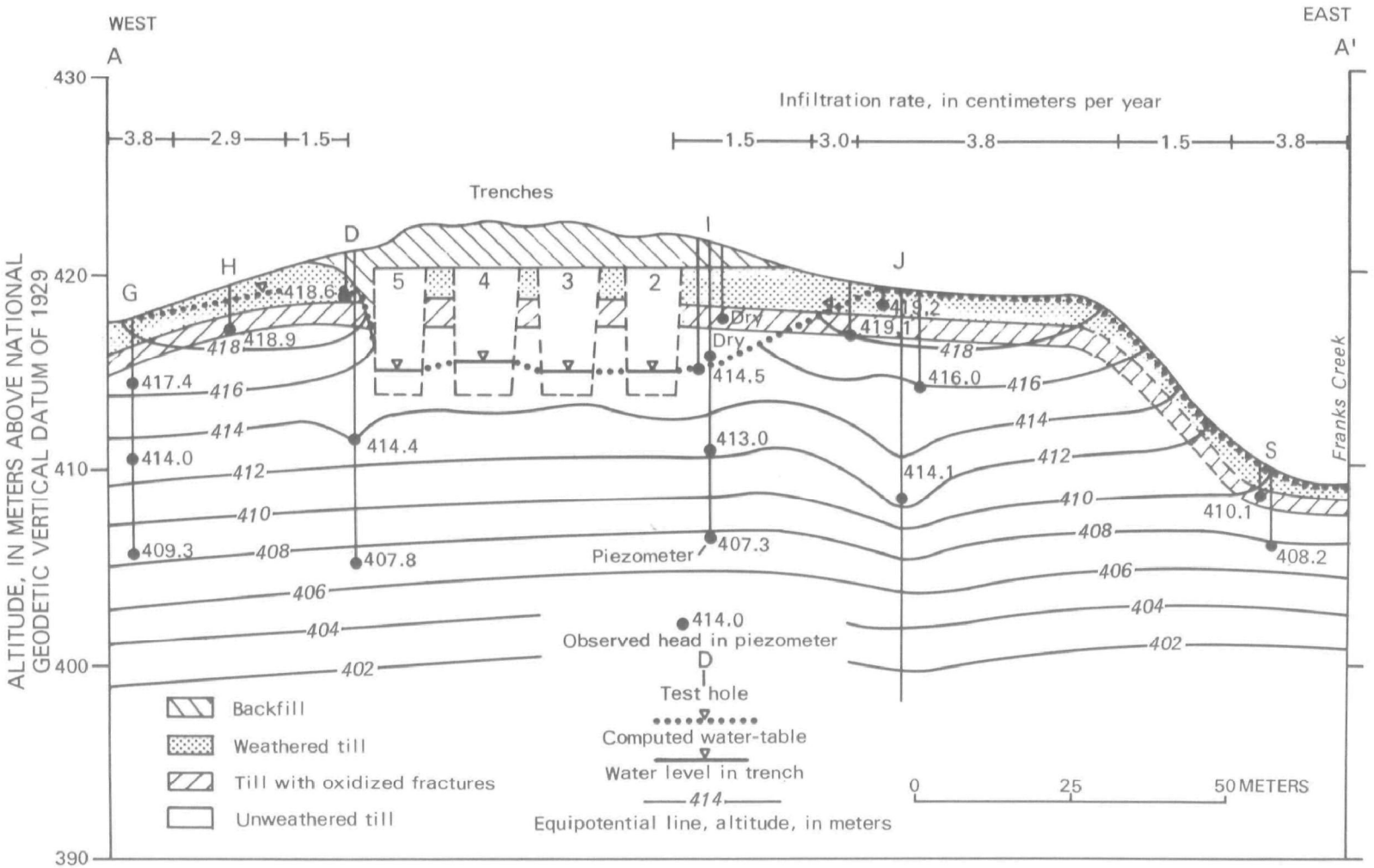

Figure 11. Cross section A-A' through north trenches showing computer-simulated distribution of head in February 1978.

However, the simulation assumed that water was instantaneously withdrawn from trench 5 to lower the water-surface altitude from 418.5 m to 416.5 m, whereas this decrease actually occurred over a 10-day period. An instantaneous drop in trench 5 water level would have caused the water level in piezometer D-1 to decline more rapidly than it did (see curve in fig. 8)); thus, a more representative value of specific storage would be between 8×10^{-6} and 12×10^{-6} cm^{-1}, which agrees well with the average value of specific storage obtained from laboratory tests. In simulations over longer periods, the best fit to the water-level declines in the deeper piezometers (D-2, F-3, E-3) were obtained when the specific-storage value of the till was near 12×10^{-6} cm^{-1}. Simulated water levels in piezometers D2-1, D-1, and D-2, based on a specific-storage value of 12×10^{-6} cm^{-1}, are compared in figure 13 to values observed during the 8 months after the pumpout of trenches 3-5. Consistent with field observations, water levels in piezometers distant from trench 5 showed no substantial declines.

As discussed previously, more than one combination of hydraulic conductivity, specific storage, and infiltration value can be used to correctly simulate head in the till after the pumpout of the trenches. However, the simulations must approximate actual flows within the till because (a) simulated and observed drawdowns in piezometers next to trench 5 are controlled more by the trench water level than by infiltration from land surface, and (b) the values of hydraulic conductivity and specific storage tested by model calibration are close to the values determined in the field and laboratory.

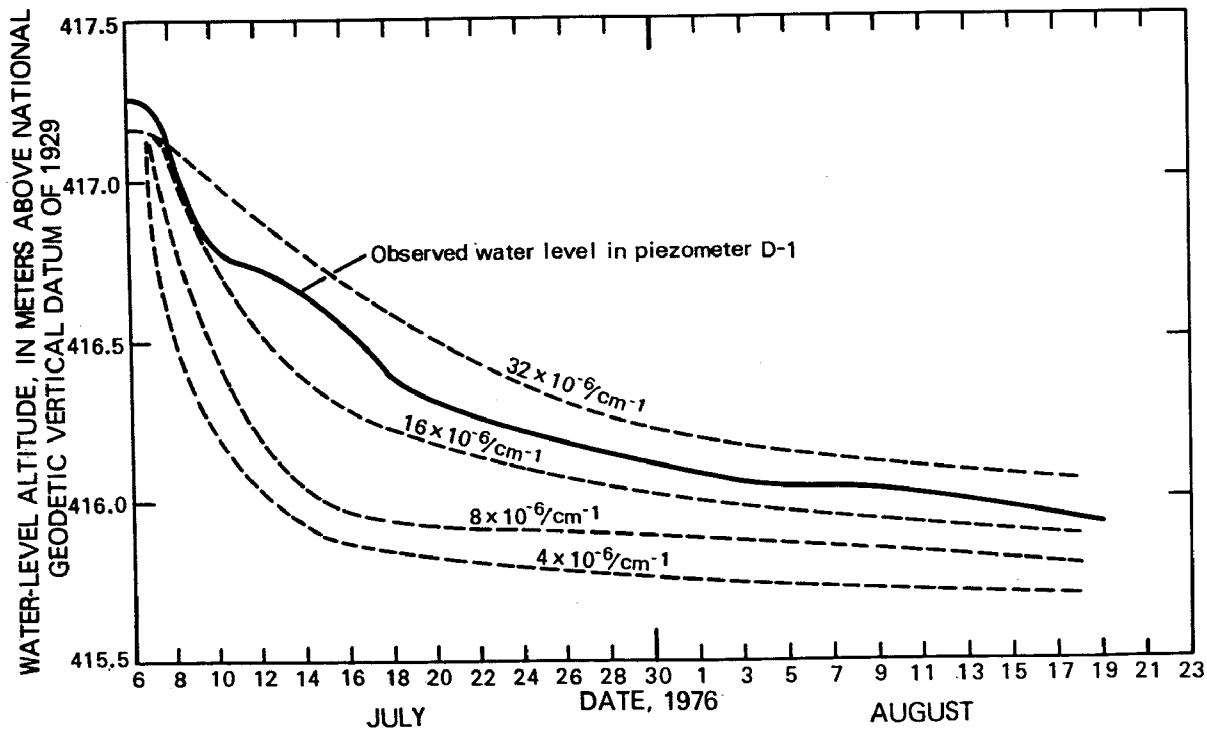

Figure 12. Comparison of observed water level in piezometer D-1, July-August 1976, with computer-generated water levels produced by changing values of specific storage.

No attempt was made to calibrate the unsaturated functions of hydraulic conductivity and volumetric soil-moisture content in relation to soil-moisture tension because the entire section is simulated with saturated or nearly saturated conditions.

After the pumpout of water from trench 5 in September 1976, water level resumed the rising trend observed before the pumpout (fig.13). Transient-state model results of the situation 25 days after the pumpout was complete showed flow into trench 5 through the till to be 0.2 cm^3/s and flow out of the trench to be 0.4 cm^3/s. (As a verification, flow out of trench 5 was manually calculated from Darcy's law to be 0.8 cm^3/s based on a hydraulic conductivity of 8×10^{-8} cm/s, a trench-floor area of 1×10^7 cm^2, and a gradient of 1:1.) The transient-state simulation also indicated that, 6 months after the pumpout, flow from the till into trench 5 had decreased to 0.1 cm^3/s. Thus, the continued rise in trench 5 water level after the pumpout was probably not caused by flow of water from the surrounding till. If the rise were caused by the slow drainage of water from less permeable zones within trench 5 that were saturated before the pumpout, the rise should have slowed with time, which was not the case after the first few days (fig. 4). Therefore, it seems likely that the rise was caused by continued infiltration of precipitation through the cover.

COMPUTER MODELING OF GROUNDWATER FLOW TO NEAREST STREAM

In general, water from the trenches moves downward through the till beneath the trench floor until it reaches the lacustrine unit 30 m below land surface; from there it should move eastward to Buttermilk Creek. However, if some of the trench water could flow to any of Buttermilk Creek's tributaries that surround the trenches, both the length of the flow path and traveltime of trench water to reach land surface would be much less. The shortest distance between a trench and an adjacent stream, and also the greatest vertical relief, is at the north end of trenches 3 and 4 (fig. 1). To evaluate this possible flow path, piezometers were installed along the slope from trench 4 to the small stream north of trench 4, in line with holes C, C2, and an older test hole (2C) that had been installed by the site operator (fig. 1).

A finite-element grid (fig. 14) was designed to represent the cross section through these piezometers, and the model was used to simulate conditions observed in February 1978. The boundary conditions were the same as those used for the section A-A', perpendicular to the north trenches (fig. 9), and values of hydraulic conductivity and specific storage were obtained from the same section. The best simulations used infiltration rates of 2 and 2.5 cm/yr along the steep slope and the smooth surface near hole 2C and C, respectively, and these rates approximate those rates used for scraped or sloping surfaces in the other section. The average absolute deviation from observed heads in seven piezometers was 14 cm. The shallow piezometer in test hole C (C-1) was simulated as dry. Computed average head value near hole 2C compares well with the observed head value, although the exact screened interval in hole 2C is uncertain.

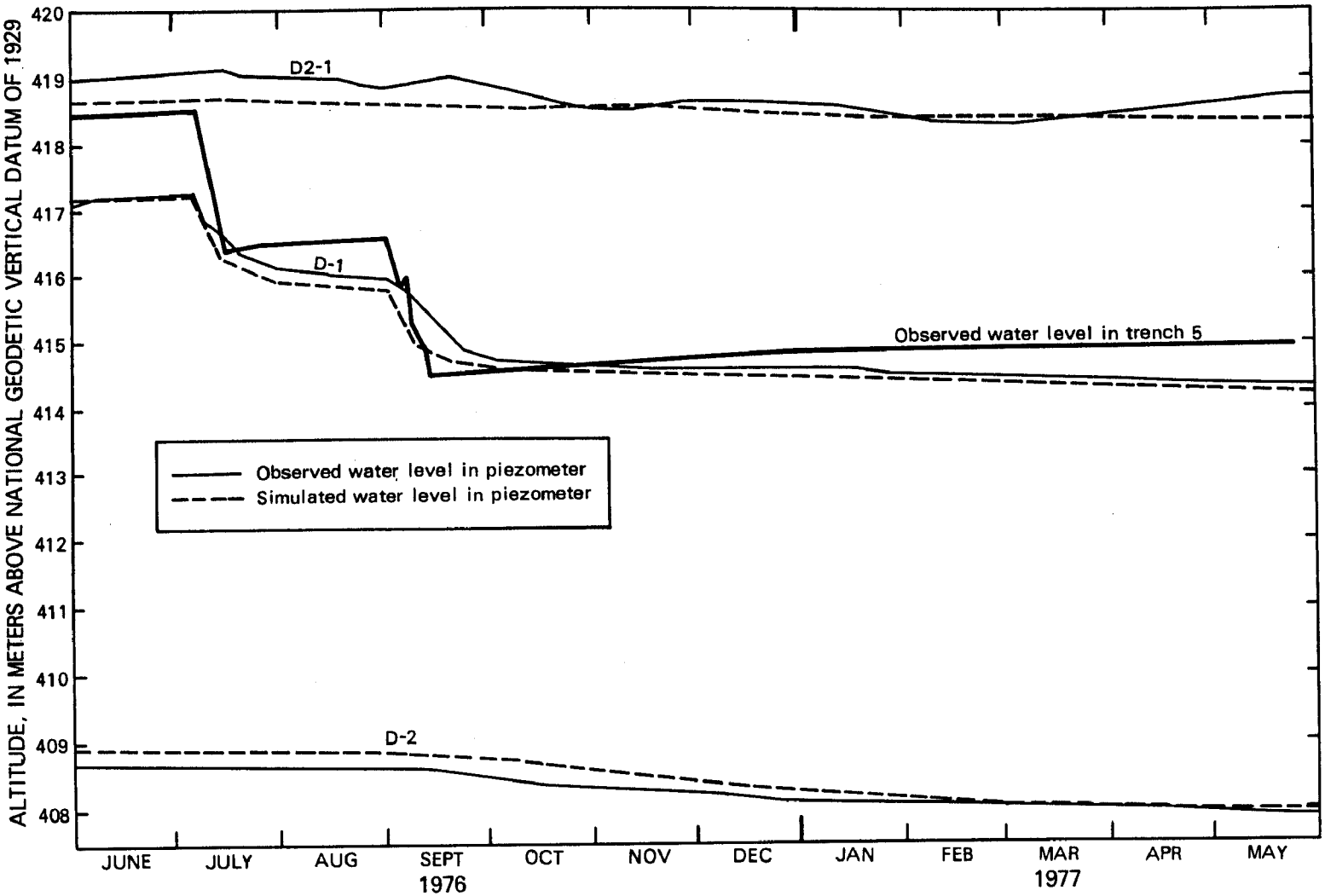

Figure 13. Comparison of computer-generated water levels with observed water levels in piezometers D-1, D-2, and D2-1 during 8 months after pumpout of water from trench 5.

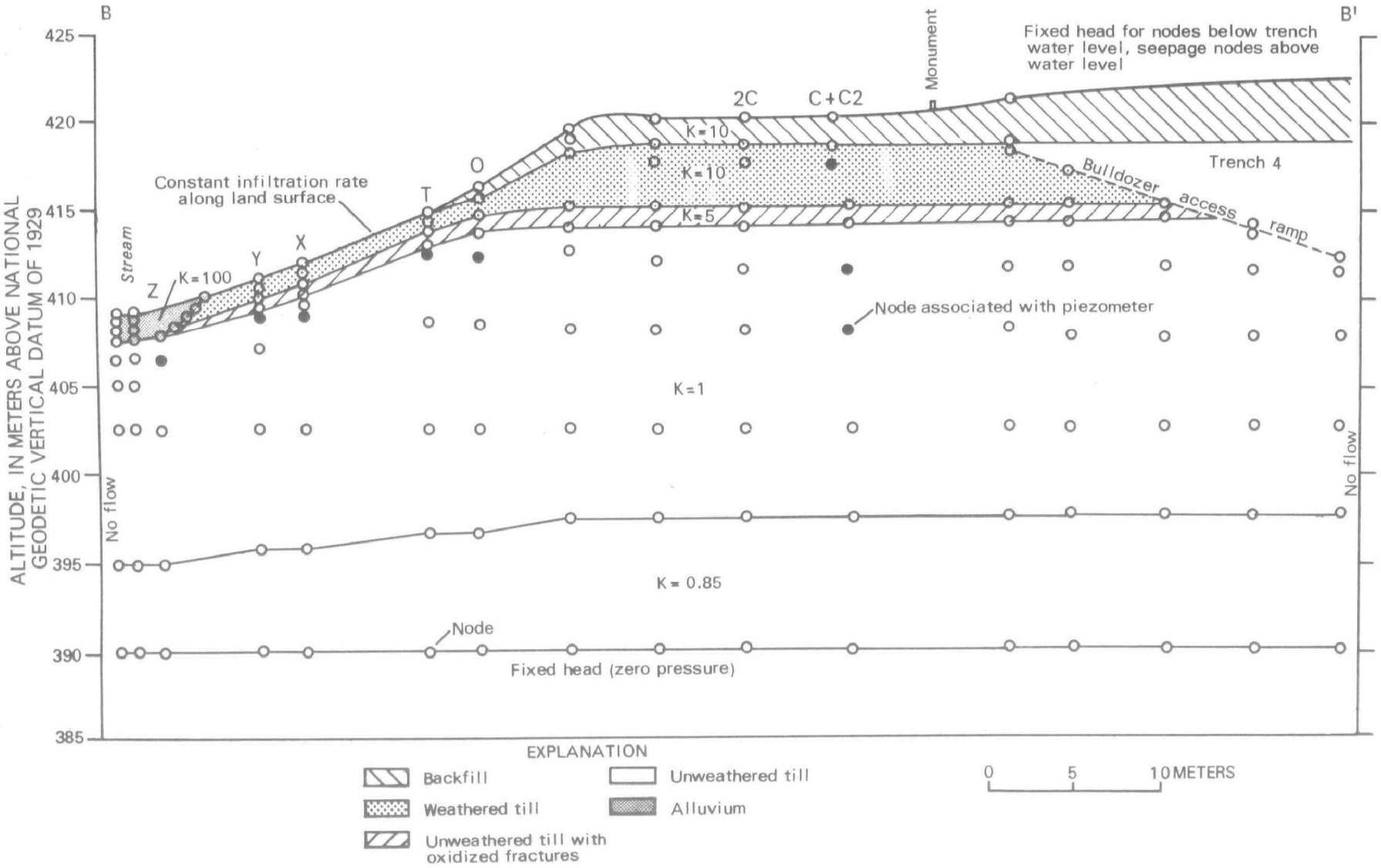

Figure 14. Cross section B-B' from trench 4 to small stream showing arrangement of nodes, boundary conditions, and relative hydraulic conductivities used in the best-fit model simulations. (Location of section is indicated in fig. 1.)

Simulation of heads for February 1976, when water level was near the top of trench 4, produced slightly positive heads in piezometer C-1, although it had been dry at this time, and simulated heads in piezometers C2-1 and C2-2 increased to almost 110 cm, or about 70 cm more than the observed increase. Increasing the hydraulic conductivity of the weathered unit in the model lowered the model heads near test holes C and C2 and increased them along the slope, but, when the lower trench-water levels of February 1978 were simulated, the decrease in piezometers C2-1 and C2-2 was still 70 cm more than the observed change.

The change in simulated heads in piezometers C2-1 and C2-2 that resulted from the lowering of model trench-water level approximated the observed change when the model trench boundary was moved to 4 m south of the monument that reportedly marks the end of the trench. (Exact location of the trench boundaries is not known; the monuments that mark the ends of trenches 1-4 were not placed immediately after completion of the trenches but after the cover over trenches 1-4 had been modified into individual mounds. Also, the ends of the trenches are sloped to allow for bulldozer access (20), but the slopes may differ from their design.) Moving the model boundary away from test holes C and C2 seemed logical in that the observed head decline in piezometers C2-1 and C2-2 was considerably less than that observed in piezometers next to trench 5. Piezometers in test hole B, finished 3 m north of the monuments on trenches 2 and 3 (fig. 1), did not show any appreciable decline in water levels after the pumpout of water from the sumps in those trenches.

The change in trench 4 water level between February 1976 and 1978 was reflected in wells 80 m and 175 m south of the north end; it is possible that the water level in the extreme north end of trench 4 did not fully respond to the pumpout of water from the sump 135 m to the south. A similar lack of response was noted in the north end of trench 5 (18), although Kelleher (2) reported that water had seeped out along the north end of trench 4 when the water level was at an altitude of 421 m. A simulation of the October 1975 water level in trench 4 (altitude 419 m) produced a slight pressure head (13 cm) in piezometer C-1, which is consistent with indications during the drilling of test holes C and C2 that a sand interval 2 cm thick, encountered at the depth of piezometer C-1, was saturated.

Simulations with the trench boundary moved 4 m south produced an average absolute deviation of 11 cm for February 1978 and 14 cm for February 1976. In both simulations, heads did not change along the slope toward the stream. The simulation of February 1978 suggests that water leaving trench 4 at that time would not move to the nearby stream and that there was a slight gradient in the water table toward trench 4 from holes 2C, C, and C2. Even when the water level approached the top of trench 4 (altitude 418 m) as in February 1976, water from the trench would move only about 8 m through the weathered till before it would move downward through the unweathered till (fig. 15).

Discharge into the stream was about 100 $(cm^3/d)/m^2$, which is similar to the values calculated for section A-A', perpendicular to the north

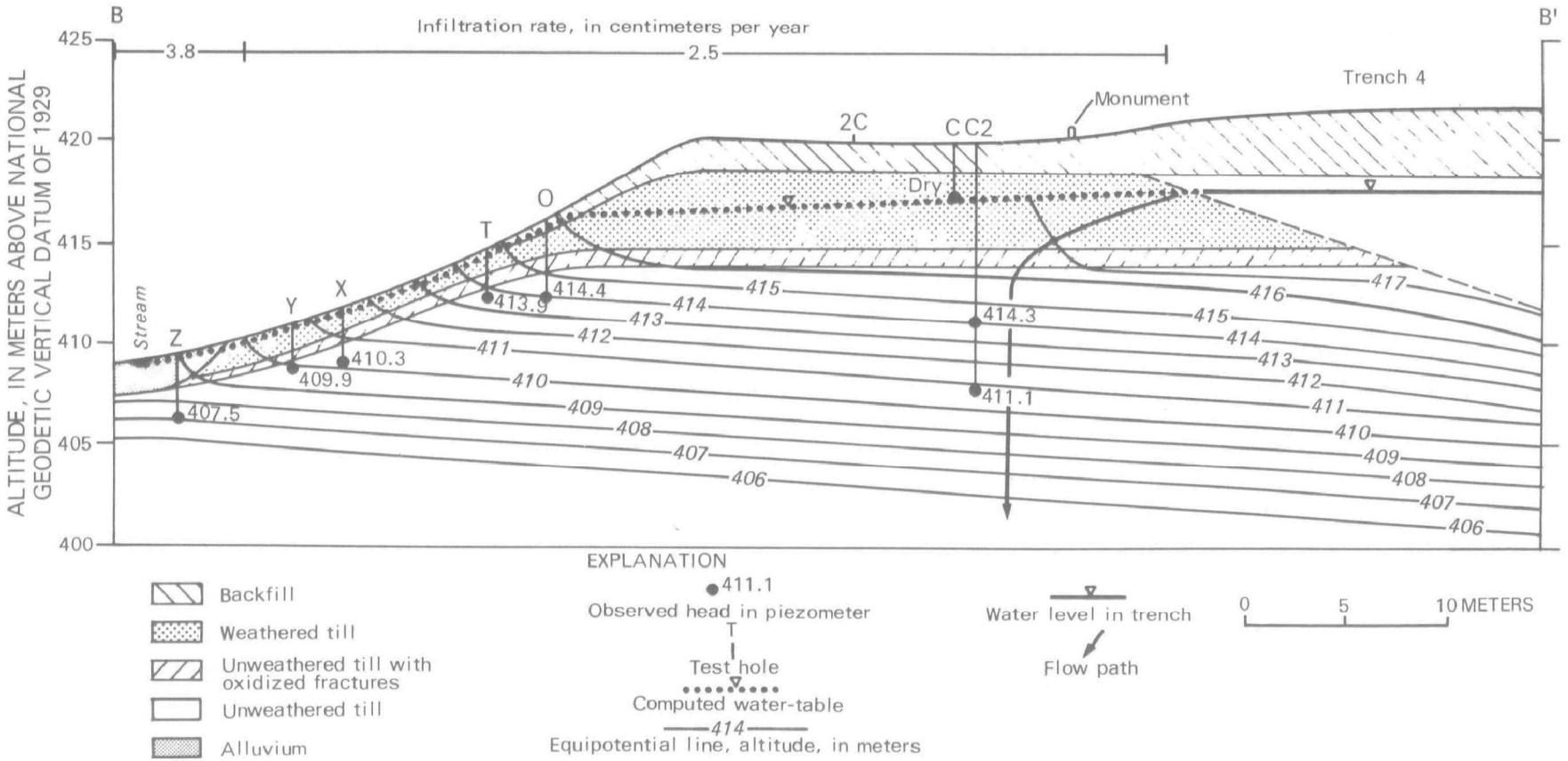

Figure 15. Computer-simulated heads along section B-B' from trench 4 to a small stream during February 1976.

burial trenches. Most of this flow was from infiltration of precipitation along the slope. The discharge rate increased by only 0.25 $(cm^3/d)/m^2$ when the simulated water level in trench 4 was increased to match the level for February 1976; this increase is attributed to the slightly higher water levels near test hole 2C.

MODEL LIMITATIONS

In general, simulated heads closely matched observed heads when silt and sand lenses of limited extent were represented. Although no continuous stratigraphic unit within the till is known that is more permeable than the till, a lens of silt and sand a few meters in length in one direction would locally alter the flow system, as conceptualized from simple modeling based on average till properties.

The simulations were based on the assumption (a) that the unweathered till has a uniform hydraulic conductivity along the sections described except for variations caused by known sand and silt lenses and by consolidation of the till from overburden, and (b) infiltration rates of swamp areas differ from those of smooth, sloping surfaces. Although the modeling results would be the same if infiltration rates were made constant along the entire section and hydraulic conductivity were increased throughout areas of lower heads. Such a change in hydraulic conductivity does not seem correct, though, because cores from swampy areas did not differ significantly from those taken from smooth, sloping surfaces and because piezometers along smooth, sloping surfaces did not consistently show higher hydraulic conductivity than those near swamps.

SUMMARY

Groundwater flow at the burial site is predominantly downward at an average rate of generally less than 3 cm/yr. Results of computer simulations support conclusions from laboratory tests and visual examination of cores that the till is generally isotropic but becomes less permeable with depth as a result of two factors: (a) fractures caused by weathering and a corresponding increase in hydraulic conductivity of the till near land surface (these fractures become less abundant with depth and are absent below 5 m), and (b) consolidation of the till by overburden pressure, which reduces intrinsic permeability progressively with depth. Simulation of four isotropic layers of differing hydraulic conductivity was an adequate representation of these factors. Hydraulic conductivity of the upper two layers (fractured till) was determined by model calibration only.

The specific storage value of the till derived from computer simulations of water-level trends in piezometers next to trench 5 was about 12×10^{-6} cm^{-1}. This is a factor of only 1.5 more than the average value obtained from four consolidation tests of core samples.

Some of the local variations in pressure head can be explained by areal differences in infiltration rates. Adequate simulations were obtained by assuming that infiltration rates on areas of smooth, sloping surfaces were about 50 percent less than the rate of 3.8 cm/yr near swampy areas.

A principal conclusion from the computer model runs is that water leaving the trenches will not intersect the nearby streams unless the trench-water levels rise to intersect the reworked till that forms the trench covers. This conclusion assumes that none of the pods of layered sediments encountered at various depths within the till are large enough to extend from a trench to a nearby stream.

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STATE-OF-THE-ART IN MODELING SOLUTE AND SEDIMENT TRANSPORT IN RIVERS

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ABSTRACT

This overview is structured around a comprehensive general model based on the conservation of mass principle as applied to dissolved and particulate constituents in rivers, with a few restricted but more specific examples that illustrate the state-of-the-art in modeling typical physical, chemical, and biological processes undergone by selected constituents in rivers. These examples include: simplified one- and two-dimensional formulations focusing on the hydrodynamic advection and dispersion mechanisms; a two-dimensional biochemical oxygen demand-dissolved oxygen model; a one-dimensional polychlorinated biphenyl model that includes uptake and release of constituent by suspended sediment, and deposition and erosion of contaminated particles; and a one-dimensional sediment transport model that accounts for interactions between the flow and the bed, and is capable of tracking dispersing slugs of sediment through cycles of erosion, entrainment, transport in suspension and as bed load, and burial and storage in the bed.

INTRODUCTION

There are many models in various stages of development that simulate one aspect or another of solute and sediment transport in rivers. I will not attempt to discuss them all or even a representative sample. There are a number of summaries, symposia, and bibliographies in the literature that do this, for example [1, 2, 3, 4, 5, 6, 7]. Rather, I will present a somewhat subjective overview that is structured first around a fairly comprehensive but nonspecific general model, and then some restricted but more specific examples that illustrate the state-of-the-art in modeling typical physical, chemical, and biological processes that are undergone by selected constituents in rivers.

Almost all mathematical models of river-transport processes are essentially accounting procedures. Nearly always they are based on the principle of conservation of one or more of the following entities:

(1) Mass of dissolved or particulate constituents, and transporting media (water, sediment particles); (2) momentum of the flowing water, which fixes the basic flow properties, including the velocity, shear stress, and pressure distributions; (3) energy, for example, thermal energy in waste-heat loading and ice-related phenomena, or kinetic and potential energy associated with fluid motion; and (4) probability, for example, accounting for the sums of probabilities in a stochastic model.

A GENERAL MODEL

The starting point for modeling solute and sediment transport processes in rivers is usually the conservation of mass principle. The other conservation principles are more likely to enter in supporting roles. The basic three-dimensional (3-D) conservation of mass equation for a dissolved or particulate constituent that is being transported by the flowing stream is:

$$\underbrace{\frac{\partial C}{\partial t} + \underbrace{\frac{\partial}{\partial x}(uC) + \frac{\partial}{\partial y}(vC) + \frac{\partial}{\partial z}(wC)}_{\text{Advection}} - \underbrace{\frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial C}{\partial z}\right)}_{\text{Turbulent diffusion}}}_{\text{Hydrodynamic}} = \underbrace{\Sigma S_i}_{\substack{\text{Internal} \\ \text{sources} \\ \text{and} \\ \text{sinks}}} \qquad \text{- - - - - - - -} \quad (1)$$

where

C = concentration of solute or particulate constituent,

x, y, z = distances in longitudinal, vertical and transverse directions,

u, v, w = time-averaged local velocities of solute or particulate constituent in x, y, z directions,

$\varepsilon_x, \varepsilon_y, \varepsilon_z$ = local coefficients of turbulent diffusion for solute or particulate constituent in x, y, z directions,

ΣS_i = sum of internal source and sink terms,

t = time.

The advection and turbulent diffusion terms on the left-hand side of Eq. (1) represent the hydrodynamic transport and mixing mechanisms that occur within the river channel. They must be known if Eq. (1) is to be solved. Usually they are estimated by some empirically based computational method or determined by measurement. It should be noted that particulate constituents, unless they consist of or behave like fine suspended sediments, cannot be assumed to have the same local velocities and turbulent diffusion coefficients as the transporting fluid. In particular, if deposition, burial, scour and re-entrainment of particulate constituents occur, an additional conservation equation

should be introduced for the material stored in the bed. Except for determination of water-surface elevation and the cross-sectional average velocity in the downstream direction, methods for solving the complete momentum and energy equations to obtain local velocities and diffusion coefficients in natural rivers are still in their infancy. This is mainly because of complications associated with irregularities of channel shape and alinement, and with the nonlinearity of the equations.

The internal source and sink terms on the right-hand side represent time rates of increase (or decrease) of solute or particulate concentration due to physical, chemical, or biological reactions and transfer processes occurring within the flow cross section. Examples of these mechanisms are radioactive decay, uptake and release of constituent by suspended sediment, photolysis, hydrolysis, oxidation-reduction reactions, bacterial degradation, and accumulation and depuration by biological organisms. The rates of these processes depend on factors such as concentrations of the constituent and substances with which it reacts, solar radiation, and variables which define the state of the aquatic environment, such as temperature, turbidity, pH, and turbulence level. External source and sink mechanisms, such as evaporative transfer, uptake and release of constituents by bottom sediments, scour and deposition of contaminated sediment, are represented as boundary conditions at the water surface or river bed and banks. The rates of these processes may depend on variables that define the state of adjacent environments, for example, wind velocity, air temperature and humidity, dynamics of flow-sediment interaction at the bed, in addition to the factors listed previously for the internal sources and sinks. Fortunately, many source/sink mechanisms can be simulated acceptably by first-order-reaction kinetic models.

If there are reactions between different constituents, or if exchange of a constituent occurs between different phases of the aquatic environment (for example, uptake and release of dissolved constituent by suspended or bottom sediments), a set of coupled equations, with one equation for each constituent and (or) phase, may be formulated. These equations, each similar to Eq. 1, are coupled by source/sink terms that specify the rates of reaction or exchange. To obtain spatial and temporal concentration distributions for the different constituents and phases, the entire system of equations must be solved. Formulations of coupled-system models for biochemical oxygen demand (BOD) and dissolved oxygen (DO), and polychlorinated biphenyls (PCB's) are presented in the next section.

SELECTED RESTRICTED FORMS OF GENERAL MODEL

Two-Dimensional and One-Dimensional Formulations

Except in the initial mixing region just downstream from a concentrated source of constituents, for example, a simple pipe outfall, adoption of 3-D models like Eq. (1) for use in rivers is rarely either justified or feasible. Firstly, substances transported by rivers tend

to become mixed, first over the depth of flow (or possibly across the channel in situations where there is persistent density stratification), and then throughout the entire channel cross section. Thus, after distances that are typically on the order of 50 to 100 times the depth and 100 to 500 times the width, the mixing can be modeled first as a two-dimensional (2-D) and eventually as a one-dimensional (1-D) process. Secondly, neither 3-D modeling of the momentum or energy equations nor any other computational method is far enough advanced to provide sufficient information about the local velocities, particularly the components normal to the mean flow, and diffusion coefficients. Thirdly, even with advances in modeling and increased computer storage capacity, complete solutions for 3-D models are likely to remain prohibitively expensive and time-consuming, except for the most idealized and simplified cases, such as uniform flow in a prismatic channel. Using integral transform methods, Cleary and Adrian [8] have obtained analytical solutions for the 3-D advection-diffusion equation with constant longitudinal velocity, zero secondary velocities, and constant diffusion coefficients, for a solute in a rectangular channel with uniform flow.

In reducing general 3-D conservation equations to simplified 2-D and 1-D forms, integrating the equations over the depth of flow and (or) across the width of the channel, with the use of appropriate boundary conditions, is preferred rather than simply neglecting the advection and diffusion terms for whatever dimension is being eliminated, and assuming for convenience that the remaining velocities and diffusion coefficients are constant throughout the depth or cross section. Following the appropriate integration procedure, one finds that some terms are eliminated naturally due to boundary conditions, and that other terms may adopt a new form in the reduced equation. Also, one is more likely to obtain correctly formulated external source/sink terms when they arise naturally from applying boundary conditions to the integrated 3-D equations. Following the concepts of Fischer [9], integration of Eq. (1) over the depth of flow leads to the 2-D conservation of mass equation:

$$\underbrace{\frac{\partial \bar{C}^d}{\partial t} + \bar{u}^d \frac{\partial \bar{C}^d}{\partial x} + \bar{w}^d \frac{\partial \bar{C}^d}{\partial z}}_{\text{Advection}} - \underbrace{\frac{1}{d}\frac{\partial}{\partial x}\left(dE_x \frac{\partial \bar{C}^d}{\partial x}\right) - \frac{1}{d}\frac{\partial}{\partial z}\left(dE_z \frac{\partial \bar{C}^d}{\partial z}\right)}_{\text{Dispersion}}$$

$$= \underbrace{\Sigma \bar{S}_i^d + \Sigma \bar{S}_e^d}_{\substack{\text{Internal} \quad \text{External} \\ \text{Sources and sinks}}} . \qquad (2)$$

Similarly, integration over the cross-sectional area leads to the 1-D formulation:

$$\underbrace{\frac{\partial \bar{C}^A}{\partial t}}_{\text{Advection}} + \underbrace{U^A \frac{\partial \bar{C}^A}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left(AK_x \frac{\partial \bar{C}^A}{\partial x}\right)}_{\text{Dispersion}} = \underbrace{\Sigma \bar{S}_i^A + \Sigma \bar{S}_e^A}_{\substack{\text{Internal} \quad \text{External} \\ \text{Sources and sinks}}} . \qquad (3)$$

In Eqs. (2) and (3) $\overline{(\ )}^{d}$ and $\overline{(\ )}^{A}$ represent averages taken over the depth, d, and the cross-sectional area, A, respectively. Also, the new coefficients E_x, E_z, and K_x no longer represent turbulent diffusion alone. They now represent longitudinal and transverse dispersion from the combined action of vertical and cross-sectional variation of the local velocities u and w and turbulent diffusion.

Formulating Eq. (2) and the depth-integrated continuity equation for water in a 2-D orthogonal curvilinear coordinate system, and replacing the transverse distance z by the transverse cumulative discharge measured from one bank

$$q_c = \int_{z_L}^{z} d\,\bar{u}^d\, m_z\, dz \tag{4}$$

leads to the stream-tube version [10] of the 2-D equation:

$$\frac{\partial \bar{C}^d}{\partial t} + \frac{\bar{u}^d}{m_x}\left[\frac{\partial \bar{C}^d}{\partial x} - \frac{\partial}{\partial q_c}\left(m_x d^2\, \bar{u}^d\, E_z\, \frac{\partial \bar{C}^d}{\partial q_c}\right)\right] = \Sigma \bar{S}_i^d + \Sigma \bar{S}_e^d\ . \tag{5}$$

A definition sketch for the coordinate system is shown in Fig. 1. Eq. (5) is more suitable than Eq. (2) for solute-transport modeling applications in natural rivers. The transverse advection term, which does not appear in Eq. (5), has been formally eliminated by introducing the continuity equation, and not simply neglected. Another advantage of Eq. (5) is that the new transverse coordinate variable, q_c, varies within a fixed range from zero to the total river discharge, Q, irrespective of whether the river meanders, or contracts and expands in width.

In Eqs. (4) and (5), m_z and m_x are metric coefficients to correct for differences in transverse and longitudinal distances resulting from curvature in channel alinement. They can be evaluated from the stream tube geometry. Except in abruptly converging or diverging sections and in sharply curved reaches, little error results from assuming that they are equal to unity. The longitudinal dispersion term containing E_x is not included in Eq. (5), because it contributes little to longitudinal dispersion in comparison to the advection term. However, there is some evidence [11, 12] that retaining the term and assigning small values of E_x helps to control troublesome overshoot problems in numerical solutions of Eqs. (2) and (5).

Finite-difference models based on Eq. (2) [11] and Eq. 5 [12] have been used successfully to simulate both unsteady and steady-state dispersion of dye and waste heat in the Missouri River. The alternating-direction implicit (ADI) method was used in both cases. Analytical solutions of a simplified steady-state form of Eq. (5) for a conservative solute, wherein the quantity $m_x d^2 \bar{u}^d E_z$ is assumed to be a constant or longitudinally varying diffusion factor, have been used with good results in a number of cases [10, 13, 14]. Analytical solutions of

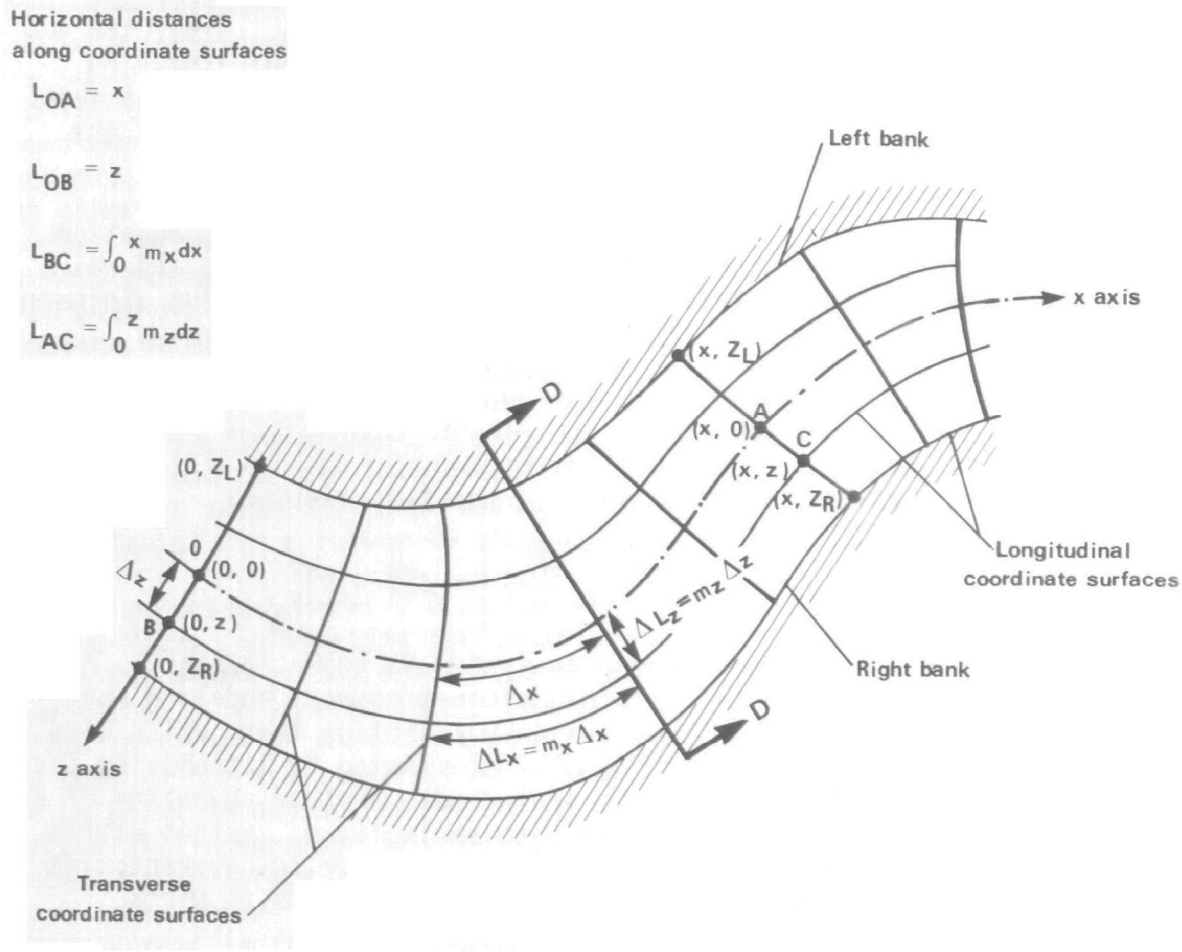

Fig. 1. Coordinate system for natural channels.

Eq. (5) also have been obtained for transient cases that have been simplified still further by assuming the channel to be straight and prismatic, and that $\bar{u}^d$ and E_x are constants [15].

Analytical and numerical solutions of the 1-D model, both with and without source/sink terms, have been widely and successfully used, especially in thermal energy (temperature) and BOD-DO models [16, 17, 18, 19, 20]. However, in modeling instantaneous concentrated-source dye experiments that simulate accidental releases of slugs of conservative soluble pollutants, significantly improved results commonly are obtained by coupling the 1-D advection-diffusion equation (Eq. (3) with no source/sink terms) for the main stream to a dead-zone equation [21, 22] as follows:

$$\frac{\partial C_m}{\partial t} + U^A \frac{\partial C_m}{\partial x} - K_x \frac{\partial^2 C_m}{\partial x^2} = - \frac{KP}{A_m} (C_m - C_d) \tag{6}$$

$$\frac{\partial C_d}{\partial t} = \frac{KP}{A_d} (C_m - C_d) \ . \tag{7}$$

The subscripts m and d denote main stream and dead zone respectively; K = coefficient for mass transfer between main stream and dead zone (in units of velocity); and P = average length of interface, in plane of cross section, between the subareas A_m and A_d. Coupling with the dead-zone equation simulates the effect of separation zones caused by bank and bed irregularities, which trap some of the dispersing material and release it slowly back into the main stream, adding to the tails, and consequently the skewness of the concentration-distribution curves, as observed in many dye experiments [23, 24]. In thermal energy and BOD-DO applications, temperature and concentrations usually change slowly enough that addition of the dead-zone equation, and often even inclusion of the longitudinal dispersion term, is unnecessary.

Two-Dimensional Biochemical Oxygen Demand-Dissolved Oxygen Model

The BOD-DO model is selected for illustration because it exemplifies a coupled-system model that includes both internal and external source/sink terms. Also, its 1-D form has a long history of successful application dating back more than 50 years to the Streeter-Phelps equations [25], the most rudimentary form of the model. The stream-tube version of the 2-D model formulated here has not yet been applied. However, the ADI finite-difference techniques used in solving Eqs. (2) and (5) should work, after modification to include the source/sink terms. The 2-D model would be appropriate for use in wide rivers, where the time scale for mixing across the channel equals or exceeds the time scales for BOD assimilation and DO replenishment.

The model consists of a coupled set of three equations for first-stage carbonaceous BOD (CBOD), nitrogenous BOD (NBOD), and dissolved oxygen (DO). In most respects, it follows Thomann's [26] 1-D formulation. The dependent variables are:

L = depth-averaged CBOD concentration, in mg/ℓ;

L^N = depth-averaged NBOD concentration, in mg/ℓ;

C = depth-averaged DO concentration, in mg/ℓ.

The three equations are:

$$\frac{\partial L}{\partial t} + \frac{\bar{u}^d}{m_x}\left(\frac{\partial L}{\partial x} - D\frac{\partial^2 L}{\partial p^2}\right) = \underbrace{-(K_d + K_s)L}_{\substack{\text{Bacterial oxidation;} \\ \text{Sedimentation, Adsorption}}} \tag{8}$$

$$\frac{\partial L^N}{\partial t} + \frac{\bar{u}^d}{m_x}\left(\frac{\partial L^N}{\partial x} - D\frac{\partial^2 L^N}{\partial p^2}\right) = \underbrace{-K_N L^N}_{\substack{\text{Bacterial} \\ \text{oxidation}}} \tag{9}$$

$$\frac{\partial C}{\partial t} + \frac{\bar{u}^d}{m_x}\left(\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial p^2}\right) = \underbrace{-K_d L - K_N L^N}_{\substack{\text{Bacterial} \\ \text{oxidation}}} + \underbrace{K_a(C_s - C)}_{\substack{\text{Surface} \\ \text{reaeration}}} \tag{10}$$

$$\underbrace{-S_B(x,p,t)}_{\substack{\text{Removal by} \\ \text{benthal} \\ \text{demand}}} + \underbrace{S_P(x,p,t)}_{\substack{\text{Production by} \\ \text{plant} \\ \text{photosynthesis}}} - \underbrace{S_R(x,p,t)}_{\substack{\text{Removal by} \\ \text{plant} \\ \text{respiration}}} .$$

On the left-hand side of the equations, $p = q_c/Q$ is the cumulative discharge normalized by the total river discharge Q, and D is the transverse diffusion factor, taken as the average value of $m_x d^2 \bar{u}^d E_z/Q^2$ and assumed to be constant across, but not necessarily along, the channel. On the right-hand side, K_d, K_s, K_N, and K_a are all first-order rate coefficients. K_d and K_N are biological-rate coefficients that depend on the properties of the oxygen-demanding pollutants and the river water. K_s relates to settling (or resuspension) and adsorption, and, consequently, to the properties of the pollutant and the turbulence in the river. The reaeration coefficient, K_a, depends on the rate of surface renewal and water temperature; it has been related to river depth and velocity, as well as temperature, by several empirical equations. C_s is the saturation concentration of DO. The functional forms of the source/sink terms S_B, S_P, and S_R are not well understood. The benthal oxygen-demand rate, S_B, relates to the aerobic decomposition of organic matter in the surface layer of bottom deposits. The net photosynthetic oxygen production rate, S_P-S_R, is highly variable and depends primarily on the amount of solar radiant energy received, and its

distribution over the river depth, nutrient concentrations, dissolved oxygen, and water temperature. Point and distributed sources of BOD, from waste outfalls, tributary inflows, runoff, and so forth, can be represented by boundary conditions at and along the banks (p=0,1).

As yet there are no operational 2-D BOD-DO computer models. However, some of the better-known computer models that are available for 1-D modeling of BOD and DO in rivers are DOSAG-1 [27]; SNOSCI and SRMSCI [28, 29]; QUAL-I [30, 31]; QUAL-II [32]; and RECEIV [33]. With the exception of DOSAG-1, these programs also can model other selected water-quality constituents.

One-Dimensional Polychlorinated Biphenyl Model

Although this model has not yet been developed beyond the initial formulation stage, it is presented here because it includes uptake and release of constituent by suspended sediment, and deposition and erosion of contaminated sediment particles. Further investigation may well indicate that some revisions, additions, or deletion of terms, and so forth, should be made. However, for the purpose of this presentation, a hypothetical chemical, say ABC, would serve about as well as PCB.

Because PCB in both dissolved and adsorbed form, together with suspended and bottom sediments, are known to be important in determining the distribution of PCB in the aquatic environment, it is appropriate to formulate a coupled-system model consisting of four equations. The dependent variables for the four equations are:

$C(x,t)$ = concentration of dissolved PCB, µg/ℓ, assumed to be constant throughout the cross section;

$M(x,t)$ = concentration of suspended sediment, mg/ℓ, assumed to be constant throughout the cross section;

$rM = C_p(x,t)$ = concentration of PCB adsorbed by suspended sediment, µg/ℓ, assumed to be constant throughout the cross section;

$r_bM_b = C_b(x,t)$ = concentration of PCB adsorbed by bottom sediment, µg/ℓ, assumed to be constant throughout the active bottom layer of thickness, $h(x)$, that is involved in the erosion-deposition process;

where

$r(x,t)$ = adsorption ratio for suspended sediment, (µg adsorbed PCB)/(mg suspended sediment), assumed to be constant throughout the cross section;

M_b = concentration of bottom sediment in active bottom layer g/ℓ, assumed to be constant;

$r_b(x,t)$ = adsorption ratio for bottom sediment, (µg adsorbed PCB)/(g bottom sediment), assumed to be constant throughout active bottom layer.

The governing equations are:

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left(AK_x\frac{\partial C}{\partial x}\right) = -K_1 CM(r_c - r) + K_2 rM + W - S_b \tag{11}$$

$$\frac{\partial}{\partial t}(rM) + U\frac{\partial}{\partial x}(rM) - \frac{1}{A}\frac{\partial}{\partial x}\left[AK_x\frac{\partial}{\partial x}(rM)\right] = K_1 CM(r_c - r) - K_2 rM + W_p - \frac{V_s}{d} rM + \gamma\frac{h}{d} r_b M_b \tag{12}$$

$$\frac{\partial M}{\partial t} + U\frac{\partial M}{\partial x} - \frac{1}{A}\frac{\partial}{\partial x}\left(AK_x\frac{\partial M}{\partial x}\right) = -\frac{V_s}{d} M + \gamma\frac{h}{d} M_b \tag{13}$$

$$\frac{\partial}{\partial t}(r_b M_b) = \frac{V_s}{h} rM - \gamma\, r_b M_b \,. \tag{14}$$

The variables t, x, U, A, and K_x, were defined previously. The remaining quantities to be defined are:

K_1 = adsorption coefficient, ℓ/μg PCB-day;

r_c = limiting adsorption ratio at full adsorptive capacity, (μg adsorbed PCB)/(mg suspended sediment);

K_2 = desorption coefficient, day^{-1};

$W(x,t)$ = rate of addition of dissolved PCB from nonpoint external sources (for example, runoff and atmospheric fallout), μg/ℓ-day, assumed to be instantaneously mixed throughout the cross section;

$S_b(x,t)$ = net rate of removal of dissolved PCB due to accumulation and depuration by biological organisms, μg/ℓ-day;

$W_p(x,t)$ = rate of addition of particulate PCB from nonpoint external sources, μg/ℓ-day, assumed to be instantaneously mixed throughout the cross section;

V_s = settling velocity of suspended sediment, m/day;

$d(x)$ = mean depth of channel, m;

γ = entrainment rate coefficient for bottom sediment, day^{-1};

$h(x)$ = mean thickness of active bottom layer involved in erosion-deposition process, m.

A definition sketch for the model is shown in Fig. 2.

Eqs. (11) through (14) are written for a particular size fraction of fine sediment, for which it is assumed that: (1) Concentration distribution of suspended sediment throughout the cross section is

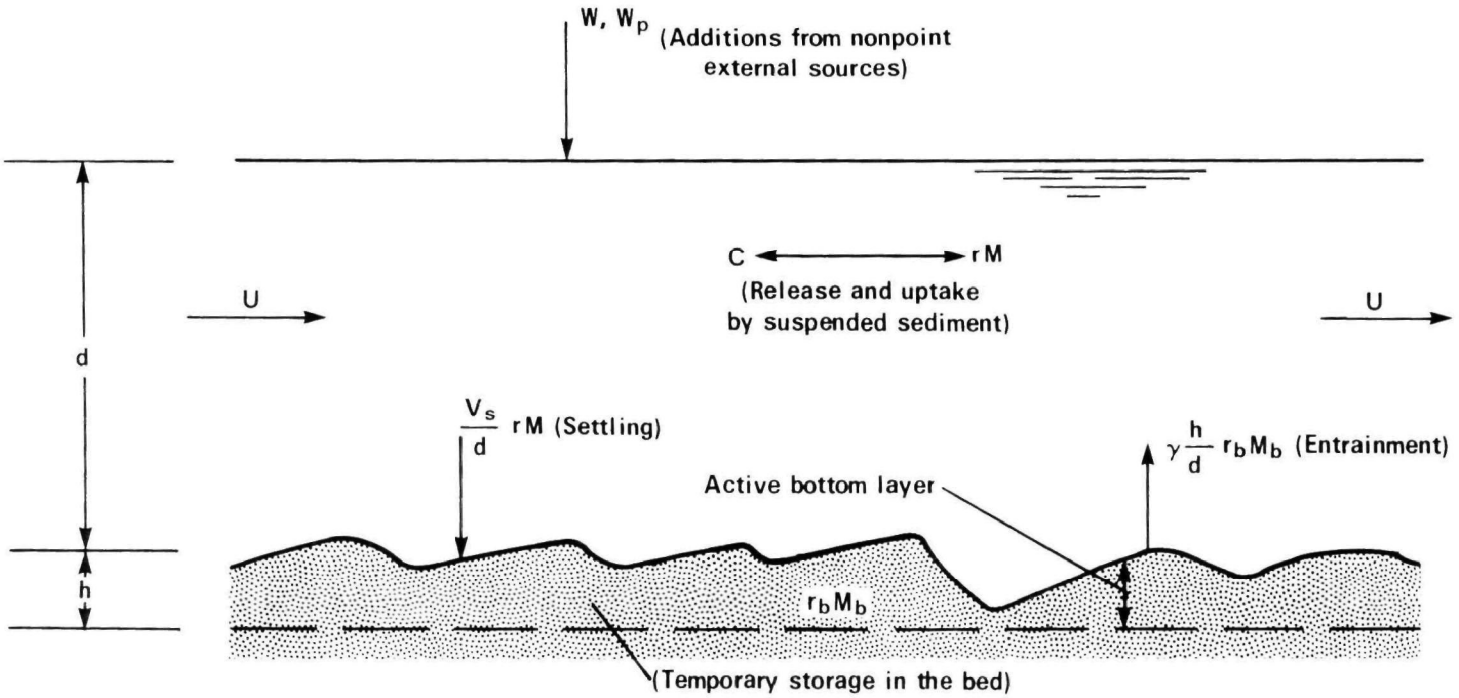

Fig. 2. Definition sketch for one-dimensional PCB model.

uniform; (2) mean velocity and longitudinal dispersion coefficient are the same as for water; and (3) settling velocity, V_s, limiting adsorption coefficient, r_c, and rate coefficients (K_1,K_2,γ) are all constants. If all size fractions are to be considered, Eqs. (12)-(14) are written separately for each size fraction, and the terms, $K_1CM(r_c-r)$ and K_2rM, in Eq. (11) are summed over all size fractions. No provisions were made in Eqs. (11) through (14) for either adsorption or desorption to occur directly between the water column and the bottom sediment, or for bedload transport. Also, an additional set of equations could be written to simulate exchange mechanisms for PCB within the bed. Such equations would be required to forecast long-term (several years) changes in PCB concentration following curtailment of its use.

Modeling of coupled sediment-contaminant systems (such as the PCB model) is still very new. The only operating models of which the writer is aware are a group of models developed by Onishi and his colleagues [34, 35, 36] at Battelle Pacific Northwest Laboratories.* These consist of 1-D and 2-D models that include equations for dissolved constituent, suspended sediment, adsorbed constituent, and exchange mechanisms that differ somewhat from those postulated in the PCB model. These models, which include both finite-element and finite-difference methods, have been used for radionuclides in the Columbia and Clinch Rivers, and for Kepone in the James River. The development of this class of models is hindered by the lack of reliable physically-based relationships and coefficients for computing rates of exchange of sediment between the active bottom layer, the bedload zone, and suspension in the flow. In addition, existing bedload transport formulas are not sufficiently reliable, except possibly for steady flow in straight uniform channels.

One-Dimensional Sediment Transport Model

The model formulated in this section exemplifies the type of sediment-transport model that needs to be developed further before the modeling of sediment-contaminant systems can come of age. In addition to predicting transport rates and hydraulic resistance, such a model would account for interactions between the flow and the bed for non-uniform and slowly-varying unsteady flow, including the development of bed forms; erosion and deposition by particle size class, possibly leading to degradation or aggradation of the bed; and changes in sediment size gradation and armoring of the bed. The model also needs to be capable of tracking dispersing slugs of sediment through cycles of erosion, entrainment, transport in suspension and as bedload, deposition, and burial and storage in the bed.

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*The use of trade name is for descriptive purposes only and does not imply endorsement by the U.S. Geological Survey.

A definition sketch for a model that meets the above requirements is shown in Fig. 3. The model consists of the following system of equations.

Equation of motion for water:

$$\frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + g \frac{\partial d}{\partial x} = g(S_o - S_f) \tag{15}$$

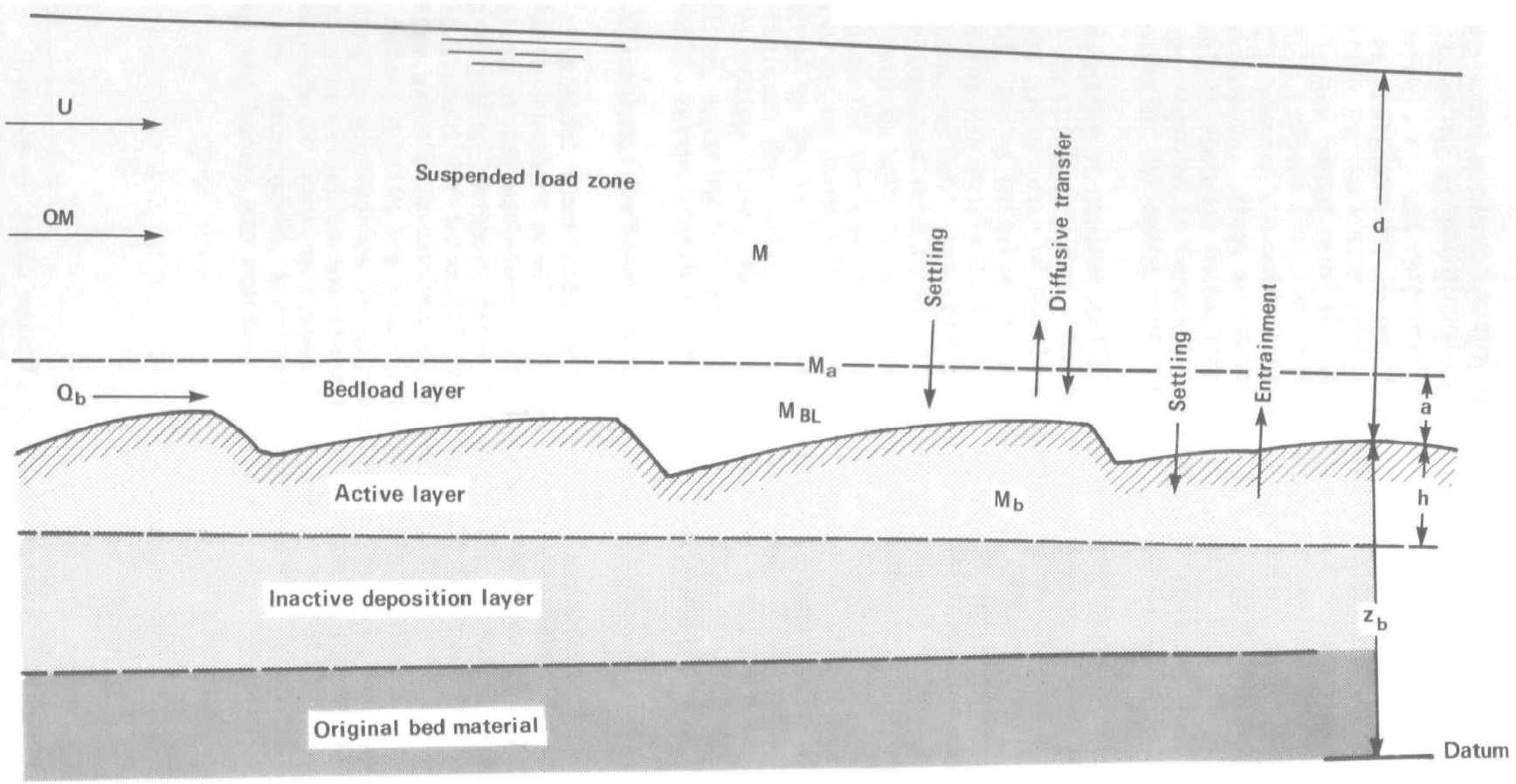

Fig. 3. Definition sketch for one-dimensional sediment transport model.

Continuity equation for water:

$$\frac{\partial A}{\partial t} + U \frac{\partial A}{\partial x} + A \frac{\partial U}{\partial x} = 0 \tag{16}$$

Continuity equation for sediment in suspended load zone:

$$\frac{\partial M}{\partial t} + U \frac{\partial M}{\partial x} - \frac{1}{A} \frac{\partial}{\partial x} \left(AK_x \frac{\partial M}{\partial x}\right) = \underbrace{-\frac{W}{A} V_s M_a}_{\text{Settling}} + \underbrace{\frac{KW}{A} (M_{BL} - M_a)}_{\text{Diffusive transfer}} \tag{17}$$

Continuity equation for sediment in bedload layer:

$$Wa \frac{\partial M_{BL}}{\partial t} + \frac{\partial Q_b}{\partial x} = \underbrace{WV_s M_a}_{\text{Settling}} - \underbrace{KW(M_{BL} - M_a)}_{\text{Diffusive transfer}}$$

$$\underbrace{-WV_s M_{BL}}_{\text{Settling}} + \underbrace{\gamma WhM_b}_{\text{Entrainment}} \tag{18}$$

Continuity equation for sediment in active bed layer:

$$\frac{W}{\rho_s} \frac{\partial m}{\partial t} = \underbrace{WV_s M_{BL}}_{\text{Settling}} - \underbrace{\gamma WhM_b}_{\text{Entrainment}} \tag{19}$$

Bedload transport:

$$Q_b = f\,(U,d,D,\ldots) \tag{20}$$

Eqs. (17)-(20), the sediment equations, are all written separately for each size fraction; following solution, the results are summed over all size fractions. The sum of the rates of change of masses, m_i, of the different size ranges of sediment in the active bed layer from Eq. (19), is related to the rate of change of bed elevation, z_b, by the equation:

$$(1-n) \frac{\partial z_b}{\partial t} = \sum_i \frac{1}{\rho_i} \frac{\partial m_i}{\partial t} \tag{21}$$

where n = porosity of the bed, and ρ_i = mass density of particles in the i-th size range.

Quantities in Eqs. (15)-(20) not heretofore defined, or with new definitions, are:

g = acceleration of gravity;

S_o = longitudinal bed slope = $\frac{\partial z_b}{\partial x}$;

S_f = friction slope determined from a hydraulic resistance equation;

M = average volumetric sediment concentration; and the subscripts a, BL and b denote, respectively: at the level a above the bed, in the bedload layer, and in the active bed layer;

W = active bed width, over which deposition or entrainment is occurring;

K = coefficient governing rate of diffusive transfer of sediment between suspended and bedload zones, in units of velocity;

γ = coefficient governing rate of entrainment of sediment from active bed layer into bedload layer, in units of reciprocal time;

D = characteristic sediment diameter.

Eq. (20) is a symbolically stated formula for bedload discharge. Any one of a number of formulas [37], or even an empirical rating relationship developed for the reach being modeled, could be used.

In addition to the system of equations (15)-(21), the model also needs to include an accounting procedure for computing and updating the size distribution of the bed material. Selective net removal of finer size fractions by erosion tends to coarsen the bed, leading to an increased resistance to erosion, or armoring, of the bed.

Probably the weakest link in the model described in the preceding paragraphs is the lack of information on the transfer and entrainment coefficients, K and γ. Capability for predicting a and h, the thicknesses of the bedload and active layers, is not much better.

The model as proposed in Eqs. (15)-(21), with the bed material accounting procedure, is a modification of the sediment transport and armoring model developed by Bennett and Nordin [38], which has been applied to reaches of the East Fork River in Wyoming, the East Fork of the Carson River in Nevada [39], and the Rio Grande River downstream from Cochiti Dam in New Mexico [40]. Significant modifications include the replacement of a single bedload-zone equation by the bedload-layer and active bed-layer equations, and modifications of the settling, diffusive transfer, and entrainment terms on the righthand sides of Eqs. (17)-(19). The Bennett-Nordin model is in some ways similar to the U.S. Army Corps of Engineers HEC-6 model [41] for simulating scour and deposition in reservoirs and rivers. However, HEC-6 neither explicitly separates the bedload from the suspended-load transport nor simulates

the exchange of sediment between suspension in the flow and storage in the bed, so that dispersing slugs of sediment can be tracked through repeated transport-deposition-burial-resuspension cycles. The Bennett-Nordin and HEC-6 models apply only to cohesionless sediment; erosion and deposition mechanisms for cohesive sediments are somewhat different. Transport models for cohesive soils have been developed by Ariathurai and Krone [42], and Odd and Owen [43].

In most instances, significant simplifications of the sediment transport model are possible. For gradually varying subcritical flow, bed transients are known to propagate at a much slower rate than either water-surface transients [2] or concentration transients for suspended or dissolved matter. If one's interest is restricted to long-term phenomena, a quasi-steady state for the liquid phase, suspended-load zone, and bedload layer can be assumed, wherein A, U, M, and M_{BL} are taken to be invariant throughout the time interval $\Delta t = x/U$, where Δt and Δx are the time and distance steps in the numerical computation. Eqs. (15) and (16) then reduce to the steady-state non-uniform flow equation for computing water surface profile [44]:

$$\frac{dd}{dx} = \frac{S_o - S_f}{1 - Fr} \tag{22}$$

where Fr is the Froude number, and the time derivative terms in Eqs. (17) and (18) are eliminated. Also, in long-term studies, the longitudinal dispersion term in Eq. (17) can be eliminated, because longitudinal dispersion in the suspended load zone is negligible in comparison to that due to storage in and resuspension from the stream bed. In situations where the changing bed geometry is of much more concern than exchanges between and distinguishing among the modes of transport in the different zones, further simplification can be achieved by combining Eq. (18) with Eq. (17) and (or) Eq. (19). This results in an equation involving transport of the total sediment load: $Q_s = QM + Q_b$.

CONCLUSIONS

This review of solute- and sediment-transport modeling in rivers concludes with an attempt at rating the state-of-the-art for various classes of models. State-of-the-art is taken here to mean mainly overall reliability in application. A steady or quasi-steady flow, for a period that is not less than the duration of one time step, throughout the reach that is being modeled, is assumed in all cases. State-of-the-art ratings on a scale of 1 to 10 (in order of improving state), assigned subjectively by the writer to various classes of models, are listed in Table 1. The classes are defined by groups of the categories of characteristics and phenomena, identified by capital letter in the listing beneath the table.

Table 1.--Subjective Rating of State-of-the-Art, on 1 to 10 Scale (in order of improving state), for Various Classes of River Transport Models

Categories[a] of Characteristics and Phenomena included in Model	1-D Model	2-D Model
A, C, E	8	7
B, C, E	8	7
B, C, E, G	7	6
B, C, F, G	6-7	4-5
B, C, F, H	6-7	3-5
B, C, F, G, H	5-7	3-5
A, D, E	6	4
B, D, E	6	4
B, D, E, G	5	3
B, D, F, G	4-5	2-4
B, D, F, H	4-5	2-4
B, D, F, G, H	3-5	2-3
A, D, F, J	5	3
B, D, F, I, J	3-4	1-2
B, D, F, H, I, J	2-3	1-2
B, D, F, G, H, I, J	2	1

[a] Listing of categories

A. Conservative constituents
B. Non-conservative constituents
C. No density (buoyancy) effects
D. Density (buoyancy) effects
E. Single system
F. Coupled system
G. Gas or heat transfer at water surface
H. Chemical/biological reactions
I. Adsorption/desorption by sediment
J. Deposition and entrainment of sediment

In the listing of categories, the designations single system and coupled system are used in the sense defined by Thomann [26]. In a single system, usually simulated by a differential equation for a single constituent, there is a functional relationship between an input (discharge of constituent at source) and a single output (concentration of constituent in river). Coupled systems are simulated by two or more differential equations, with interacting source/sink terms.

Neither the categories nor the groupings listed in the table purport to be exhaustive. However, they do represent a large proportion of present river-transport models.

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AN OVERVIEW OF RESUSPENSION MODELS: APPLICATION TO LOW-LEVEL WASTE MANAGEMENT

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ABSTRACT

Resuspension is one of the potential pathways to man for radioactive or chemical contaminants that are in the biosphere. In waste management, spills or other surface contamination can serve as a source for resuspension during the operational phase. After the low-level waste disposal area is closed, radioactive materials can be brought to the surface by animals or insects or, in the long term, the surface can be removed by erosion. Any of these methods expose the material to resuspension in the atmosphere. Intrusion into the waste mass can produce resuspension of potential hazard to the intruder. Removal of items from the waste mass by scavengers or archeologists can result in potential resuspension exposure to others handling or working with the object. The ways in which resuspension can occur are wind resuspension, mechanical resuspension and local resuspension. While methods of predicting exposure are not accurate, they include the use of the resuspension factor, the resuspension rate and mass loading of the air.

INTRODUCTION

Resuspension and inhalation of the resuspended material is a potential pathway whereby radioactive materials can be transferred from the ground, or other surface, to man. In general, it is of greatest importance for those radionuclides that are strongly discriminated against in the food pathway. If the radionuclides are strongly taken up by foods, and food from the contaminated area is used, the contribution to the dose from resuspension and inhalation is usually small.

In this paper, we discuss the application of this pathway to the management of low level wastes and describe briefly some of the methods of estimating air concentrations from resuspended material. More detailed discussions of the technical details are available in the literature [1,2].

RESUSPENSION

Before entertaining the question of how resuspension is involved in low-level waste management, let us consider what resuspension is. Technically, it is the suspension of a material in a fluid after this material has once been deposited on a surface from a previous suspension. Thus, resuspension. This fluid can be either air or water and resuspension in both can be of importance in analyzing potential problems from low-level wastes. Air suspension is used in estimating quantities inhaled and water suspension is important in the movement of radioactive particles in streams or other bodies of water. However, for this discussion, we will confine our attention to the problem of suspension in air.

It should be apparent that not all sources meet the technical definition of resuspension given above. For example, if a radioactive material is spilled on the surface or if it moves upward to the surface, it has not been deposited by a previous suspension and should not really be considered as resuspension. However, because the mechanisms for suspension are similar regardless of the method of contamination, it is convenient to change the definition to include all cases in which the material becomes airborne from the surface.

It should also be made clear that the suspensions that we are concerned with are not the true colloidal suspensions that the chemists are used to but, rather, are particles kept in suspension by the turbulent movement of the fluid in which they are carried. Thus, an aerosol resulting from resuspended materials can contain much larger particles than could be indefinitely suspended in still air. In fact, those of you who have been caught in sand storms with strong winds will realize that large particles that can sting when they hit can be carried under conditions of highly turbulent winds.

RESUSPENSION AND LOW-LEVEL WASTES

Now, how does resuspension fit into the analysis of low-level waste? Obviously, if we do our jobs perfectly it will not become a factor. There are, however, complications such as accidents or spills that must be considered and accounted for as well as a few potential complications that could arise with the long-term behaviour of the burial grounds.

In figure 1, we find an elementary schematic drawing of a few ways that people can be exposed from low level waste operations. A number of the pathways to man have no connection with resuspension but I have included some of these as dotted boxes and lines for the sake of completeness.

The transport accidents and spills can result in contaminated surfaces that can give rise to resuspension and inhalation of

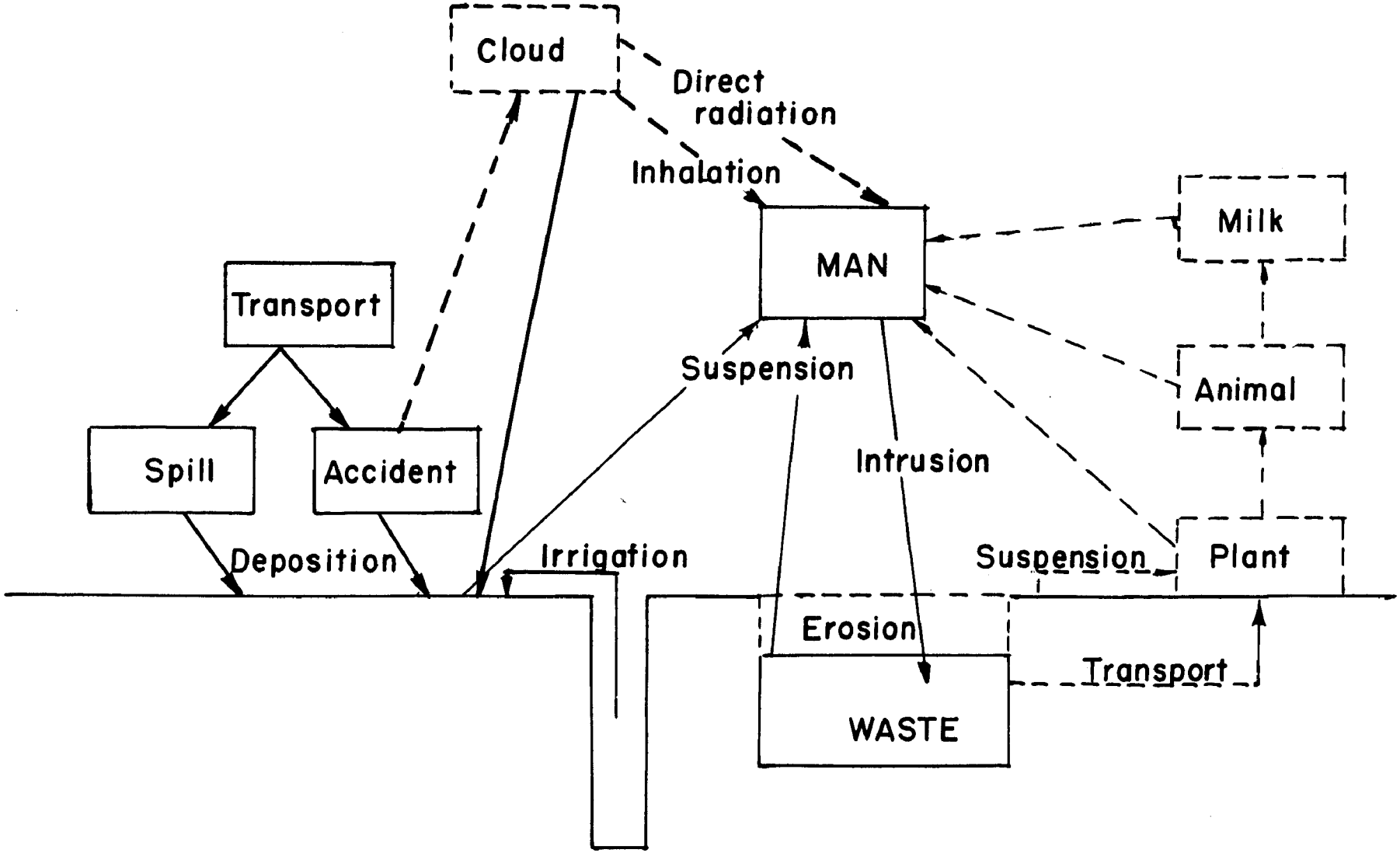

Fig. 1. Schematic drawing of pathways to man from low-level waste operations. Solid lines are related to resuspension while dotted lines are other pathways.

radioactive materials by man. These, however, should be of relatively minor concern, from the resuspension point of view, because they are usually noted and the area cleaned before serious resuspension can occur. There may be some long-term build-up of activity at places such as loading docks where the material could be resuspended, but this problem can be controlled by monitoring. These potential problems are encountered in the operational phase of the disposal area and can be handled by "institutional" methods because the workers are already there.

However, there are later opportunities for movement of radioactivity to surfaces where resuspension could be a factor. Some of these are shown in Fig. 1. For example, transport of the activity to the surface by water, ants, burrowing mammals or other means can produce a source exposed to winds or other disturbances, that could result in resuspension. The possibility that could expose the largest number of people to small quantities starts with transport to an aquifer. The water from this aquifer could be withdrawn from wells and used for irrigation, with the radioactive materials adsorbing on clays or humus to gradually produce large contaminated areas. If the aquifer empties into a stream, radioactive materials will accumulate in sediments which can be deposited on flood plains or the water can be used for irrigation with the same result as the use of well water. One aspect of resuspension in these cases which leads to the food pathway is the resuspension and deposition on food plants. Experience with nuclides that are only poorly taken up by plants indicates that this can be an important factor.

Another series of pathways involving resuspension occurs in disposal areas containing long-lived radionuclides. Here we can postulate eventual removal of the cover material by erosion, either by wind or water. When this occurs, we are left with a contaminated area to depths of several meters, augmented by surface contamination in the surrounding area caused by the materials removed and carried downwind or downstream. This radioactive material can be resuspended by winds or by movement in the area. This is a futuristic scenario depending upon the particular site of disposal. With average erosion rates, it could occur some thousands or tens of thousands of years from now although gully erosion could occur much faster but on a limited scale. In some areas, the net erosion pattern is such that the disposal area will be simply buried deeper, but the present tendency to look for areas that are "high and dry" to site disposal areas could eliminate this possibility because the high sites with a long distance to the water table are just those that will have a negative-gain erosion potential.

The intrusion case, i.e. where an individual digs into an area, either knowingly or unknowingly, results in resuspension caused by his activities. In an enclosed space this can result in high concentrations of dust and associated radioactive materials with the individual inhaling these materials. However, this exposure will be limited to the

individual or individuals concerned unless contaminated items or materials are removed and taken to a place where others can be involved.

This possibility brings up the case in which an archeologist, either amateur or professional, investigates these disposal areas for "treasures" of the past. Old burial grounds are the source of much of our knowledge of the prehistoric past and they serve as magnets to draw those interested in history. We hope that the level of knowledge in the future will be such that proper precautions are taken when this event does occur, but this is just the type of point that we cannot assure without surveillance of disposal areas until the radionuclides have decayed. Obviously any contamination on any objects removed could serve as a source of resuspension and inhalation by any individual who handles or works with these objects.

One special case in this category results from the current practice of using non-degradable plastics to contain the contamination during handling of the wastes en route to the disposal area. Current information gives little reason to believe that these plastics will not preserve their contents and remain intact under the conditions of burial in the soil. This raises the possibility of recovery of such packages with consequent exposure when the package is opened.

CLASSES OF RESUSPENSION

We have divided the overall resuspension problem into three classes defined by both their characteristics and the information needed to solve them.

The first class is wind resuspension. This occurs when the wind blowing over a field resuspends particles and moves them downwind. Much is known about the mechanics of this class through the many studies of wind erosion of agricultural fields. In essence, there is little suspension of soil particles unless a phenomenon called "saltation" occurs. Here, particles on the order of 100-200 μm in diameter start rolling over the surface and then jump into the air under the pressure of the wind. They, then, travel forward with the wind, gaining energy and meanwhile falling under the force of gravity, until they impact on the ground. This impact dislodges other smaller particles that are suspended in the air. Such a process will start at the edge of a field and increase in intensity downwind until a maximum is reached. One other process for wind resuspension, that has not been well investigated could result from the deposition of an aerosol on vegetation. Presumably any of this material that is not bound to the foliage by adsorption or absorption could be dislodged by movement of the foliage under the action of the wind.

The second class of resuspension is that caused by mechanical disturbance of the soil with the resuspended particles moving downwind to expose people. This could be, for example, a farmer plowing a field

or people walking or working and disturbing the soil. The familiar dust cloud raised by such activities in dry weather is a sign of such resuspension. Here the forces required for resuspension come from the activity but the movement, once the material is in the air, is dependent upon the winds. Many such disturbances are point sources at the point of disturbance rather than a broad area source as with wind resuspension. Another difference between these two classes is the depth to which the disturbance reaches. In wind resuspension the depth from which resuspension can occur is dependent upon the depth reached by the saltating particle or fairly shallow. In mechanical disturbance the depth can be inches or even feet depending upon the type of disturbance. Thus a source at greater depth can be resuspended than occurs with winds.

The final class is local resuspension. This is the resuspension leading to a cloud in the immediate vicinity of an individual causing the disturbance. It can apply to an individual handling a contaminated object, to an individual digging a hole in contaminated soil or to the dust cloud surrounding a farmer plowing a field. Whereas the concern with the previous two classes was with people downwind from the source of the resuspension, the concern with this class is with the individual causing the disturbance.

EVALUATION OF RESUSPENSION

Now that we have pointed out some of the ways in which the resuspension pathway to man can be of interest to low-level waste disposal, how can we evaluate its seriousness? In other words, if we can define a source term how can we evaluate the potential exposure to man? The only proper answer at this time is that we do it with considerable uncertainty and with many assumptions. Unfortunately, the studies required to better understand these problems and to obtain adequate coefficients for use are not well funded.

There are three methods, or models, for estimating resuspension: the resuspension factor, the resuspension rate and the mass loading of dust in the air.

The resuspension factor is defined as the ratio of the air concentration resulting from resuspension to the quantity of contaminant per unit area at the location where the air sample was taken. Usually, the air concentration is in activity per m^3 and the ground contamination is in activity per m^2. Thus, the units of the resuspension factor are m^{-1}. There are many values of the resuspension factor in the literature because it has been the most widely used method for many years and measurements are relatively simple. Typical of these values are those in a table by Mishina [3]. In this table, the values vary over about 10 order of magnitude. However, closer examination of this table shows that wind resuspension with freshly deposited material is in the range of 10^{-8} to 2×10^{-6} m^{-1} and for aged deposits from 6×10^{-10} to 10^{-13} m^{-1}.

For mechanical disturbance the range seems to be from 2×10^{-6} to 7×10^{-5} m^{-1}. However, many of these tests were done in arid country and may not be typical of other areas.

A decrease in the resuspension with time can be expected following deposition from the atmosphere. This decrease is caused by penetration of the contaminant into the soil or by other means of fixation, such as adsorption on large soil particles. Initially, rather crude measurements at the Nevada Test Site indicated a decrease with a half life of about one month [4]. However, as information has accumulated, it is apparent that any decrease with time is over a much longer period of time than one month. Anspaugh [5] has formulated a relation in which the resuspension is initially 10^{-4} m^{-1} with a decrease over a period of several years to 10^{-9} m^{-1}. It should be stressed, however, that such a relation is based upon meager data obtained in only one area. It may also be noted that such a decrease with time will probably not occur for other types of deposition such as liquid spills or contaminants brought to the surface from a below grade disposal site because these actions result in an initial mixing of the contaminant with the soil.

The resuspension factor has conceptual problems when it is used for describing wind or mechanical resuspension. For example, it does not account for resuspension that occurs upwind. It is primarily an empirical concept with little hope of eventually describing the important variables involved in resuspension. However, from a practical standpoint, most of the past measurements have been made using this method of interpretation so that some data are available. The resuspension factor, or some variation of it, may also be a likely choice in describing local resuspension because the receptor and the source of contamination in the air are at the same place.

The second method of describing resuspension is through the use of the resuspension rate. The resuspension rate is the fraction of the contaminant in the ground that is resuspended per unit time. This rate describes a source term that can be used with the known correlations for meterological dispersion to estimate the air concentrations of the contaminant downwind. There are not many measurements of the resuspension rate available. Sehemel [6] using a nonradioactive contaminant, measured values of 10^{-11} to 10^{-7} sec^{-1} for wind resuspension in a lightly vegetated area. Anspaugh et al. [7] measured values of 3×10^{-12} to 10^{-9} for wind resuspension in an area at the Nevada Test Site. For mechanical resuspension values of 1×10^{-16} to 1×10^{-15} sec^{-1} for an individual walking in a contaminated asphalt highway have been inferred [2] from measurements made by Sehmel [8]. For a truck driving through a tracer on an asphalt highway Sehmel [9] reports values equivalent to rates of 10^{-8} to 8×10^{-3} sec^{-1} with the resuspension rate varying with the speed of the vehicle.

The resuspension rate is plagued with the difficulty that too few measurements have been made to allow use for types of soils and in areas different than those in which measurements have been made. It also

requires knowledge of the pattern of contamination on or in the soils of the contaminated area. However, it does provide additional detail on the meaning of the measurements and, as information increases, may well be the method of choice for specific areas. It s value in studying the phenomenon of resuspension is illustrated by the findings in the past few years that the rate of resuspension increases with the wind speed at rates up to the 8th power of the wind speed depending upon the type of soil [10].

The third method for calculating resuspension is the mass loading approach. Here it is assumed that the dust in the air has the same concentration of contaminants as occurs in the soils. Anspaugh et al [11] have collected information from a number of sources and have shown that reasonable agreement between measured and calculated concentrations can be had if one assumes, for the calculation, that the concentration of dust in the air is 100 ug per m^3. Since it is doubtful that the actual concentration is this high, this finding should be regarded as a correlation rather than as a true relation between actual dust and concentration of contaminant.

There are problems with this concept also in that the measured mass loading at a given point depends upon the dust which could have arisen from a large distance upwind and would serve to dilute the dust from the contaminated area, particularly if the contaminated area is small. There have also been questions raised as to the source of the dust from the soil. That is, if the soil contains a large fraction of smaller particles which contain all of the activity, the concentration in this fraction is the one that should be used in the calculations. One investigator [12] has gone so far as to destroy all of the natural aggregates in the soil and to use the concentration in the remaining small particles which do not exist in nature, as the basis of the calculation. However, all correction factors suggested for this effect using the particle size distribution in natural soil have been comparatively small, less than a factor of two. The use of the mass loading has certain value, however, particularly in view of the correlation mentioned earlier. It should be noted that this correlation was obtained on ambient air with no disturbances in the vicinity. Thus, if it is to be used, the mass loading should be increased by some factor to allow for the possibility of mechanical disturbance. We believe that the mass loading may be the best method for generic studies not tied to a specific site.

DISCUSSION

This has been a very brief discussion of the role of resuspension in low level waste management. Other references are available that will provide additional detail [1,2]. However, it is apparent that the information available is not really adequate to do more than make a crude estimate of the inhalation problem from any of the three classes of resuspension. Additional studies, providing both basic

understandings of the mechanisms of wind resuspension and empirical data tied to specific types of areas and actions are needed to provide data for better estimates.

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AN OVERVIEW OF EPA'S HEALTH RISK ASSESSMENT MODEL FOR THE SHALLOW LAND DISPOSAL OF LLW

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ABSTRACT

EPA is developing a generally applicable environmental standard for managing and disposing of LLW as part of the National Radioactive Waste Management Program. To support the LLW standard, EPA will assess potential impacts from disposing of LLW by a number of alternatives including estimating potential releases to the environment, doses, health risks and costs from eight land disposal methods. This paper presents an overview of EPA's assessment model for shallow land disposal (SLD) of LLW. It describes model design considerations, conceptual design of model and approach to developing model. The SLD model has data preparation and main calculational sections. The main calculational section has release, transport and dose/health submodels including leaching, release, groundwater transport, surface water transport, atmospheric transport, resuspension, irrigation, operational spillage, human intrusion, biological uptake by man, dose and health risk submodels. Where possible, existing models/submodels were used. However, new submodels were developed for infiltration, leaching, release and groundwater transport. Basic system equations and brief explanations of these four submodels are given.

INTRODUCTION

The Environmental Protection Agency (EPA) is developing a generally applicable environmental standard for the management and disposal of low-level radioactive wastes (LLW) as part of the U.S. National Radioactive Waste Management Program.(1,2,3) The President has directed EPA to accelerate development of its standard.(3) The current schedule calls for EPA to issue a proposed LLW standard in September, 1982, and to publish a final LLW standard in January, 1984.

The EPA's program to develop the LLW standard includes assessing the health risks from disposing of LLW by shallow land disposal (SLD) and by other alternative disposal methods. The potential costs and benefits (reductions in health risks) from using each of these alternatives will also be compared. This information will provide input to and support for EPA's decisions concerning the standard. The analyses will also be used to fulfill the requirements of NEPA, the Environmental Impact Statement and the Regulatory Analysis.

The EPA has guidance from a number of sources on how to develop the LLW standard. These include NEPA (4), EPA's Improving Government Regulations (5), BIER II (6), Decision Making in EPA (7), ICRP 26 (8), and EPA's proposed Criteria for Radioactive Waste Management (9). These guidelines advise EPA to:

- compare the health risk and cost of reasonable alternatives;
- ensure that the health risk from the activity is acceptable;
- ensure that the health risk is as low as reasonably achievable, taking into account social and economic factors (ALARA); and
- use predetermined model(s) to make the above assessments.

The above guides clearly establish EPA's use of models to support the development of standards. Models for estimating the health risks, making the benefit/cost analyses and comparing the alternatives will be necessary for the LLW standard. The purpose of these models is to assess and predict the potential future impacts from managing and disposing of LLW by a number of realistic alternatives. These assessments will include estimating the potential releases of radionuclides to the environment and the subsequent doses, health risks and associated costs.

The focus of this paper is on EPA's environmental assessment model to simulate the health risks from disposing of LLW by shallow land disposal methods (SLD model). The general design and layout of EPA's SLD model was done in-house and a preliminary report on it was presented in February, 1979.(10) This report included a general description of the model's data input requirements, the pathways, scenarios and land disposal alternatives to be considered, and its potential applications. Specific guidance for development of the SLD model, with particular attention to the infiltration, leaching, release and groundwater transport submodels, were developed in-house by Hung and other ORP staff.(11) Since then, Hung has developed a groundwater transport submodel for the SLD model (12), and a method for characterizing the long term leachability of solidified

radioactive waste.(13) The SLD model is currently being developed by the Oak Ridge National Laboratory under an interagency agreement with the U.S. Department of Energy. It is expected that the assessment model for other land disposal alternatives can be adapted from the basic SLD model without major modifications.

CONCEPTUAL MODEL DESIGN AND DEVELOPMENT

Model Design Considerations

The following considerations influenced the design of EPA's SLD assessment model and its submodels.

- A generic model is required because EPA will be analyzing the potential impact of disposing of a wide variety of waste types by different disposal methods under sharply different hydrogeologic and climatic conditions.
- A land disposal facility should be modeled as a complete disposal system which includes the wastes, the site geology, hydrology, and climate, and all the pathways from it because the performance of the system will change if changes are made to any of its parts.
- A systems approach is needed to evaluate the effectiveness of each disposal system and proposed changes in its design (i.e., modifying the waste form or packaging).
- The model should be modular in construction to allow substitution or modification of submodels when it is used to analyze different disposal systems and sufficiently flexible to analyze disposal systems with a wide range of hydrogeologic and climatic conditions.
- A simple, one-dimensional analytical approach would be adequate and, in fact, preferred for EPA's risk assessment modeling needs to keep computer time and costs within reasonable bounds, to avoid potential errors in the numerical approach, to stay within the quality of the input data currently available, and to utilize and stay within the state-of-the-art modeling for many pathways.

Conceptual Model Design

The conceptual model for the environmental assessment of SLD consists of a group of preparation submodels group and the main calculational model. The main calculational model includes the leaching, release and environmental transport submodels and

simplified individual and population dose and health risk submodels. A block diagram of the general layout of the SLD model is given in Figure 1.

The preparation submodels prepare secondary input data for use in the main calculational model. These secondary input data are independent of the time of simulation and can be processed prior to being integrated into the main calculational model (i.e., annual rate of infiltration, health effects conversion factors, unit response of region to a release). The purpose of the preparation submodels is to prepare files of these data (i.e., annualized synthetic hydrological or meteorological conditions or other appropriate basis) as efficiently as possible, for input into the calculational submodels, thus reducing central processing unit time and costs.

The submodels within the main calculational model simulate the release and transport of radionuclides from the waste by a driving force due either to natural processes or to human activities. The transport submodels include: leaching; release; groundwater transport; surface water transport; atmospheric transport; resuspension; irrigation; operational spillage; human intrusion, including farming on the site; and biological uptake by man including food chain, drinking water, inhalation, and direct irradiation.

Water is considered to be the most important driving force for releasing radionuclides from the waste. The predominant release modes are expected to be leaching, erosion, gas generation, and human intrusion. When the radionculides are released from a burial trench, they will be available for transport to environmental receptors. The receptors considered are groundwater, surface water, air, and land surface. The main model simulates the transport of the radionuclides released among these receptors. The resultant accumulation of radionuclides in the receptors are then available for biological uptake by humans through the food chain, drinking water, inhalation, and direct irradiation pathways.

The results of these simulations furnish input into the dose and health risk submodels. The dose submodel integrates the total doses from the total radionculide uptake by humans from all critical pathways to provide an estimate of potential individual dose. The health risk submodel evaluates the corresponding health effects and integrates them over the affected population to obtain the potential total fatal health effects and number of years of life lost.

Approach to Model Development

Development of our conceptual SLD assessment model into a working model was guided by the considerations discussed earlier and the need to develop it within a relatively short time. To meet our schedule,

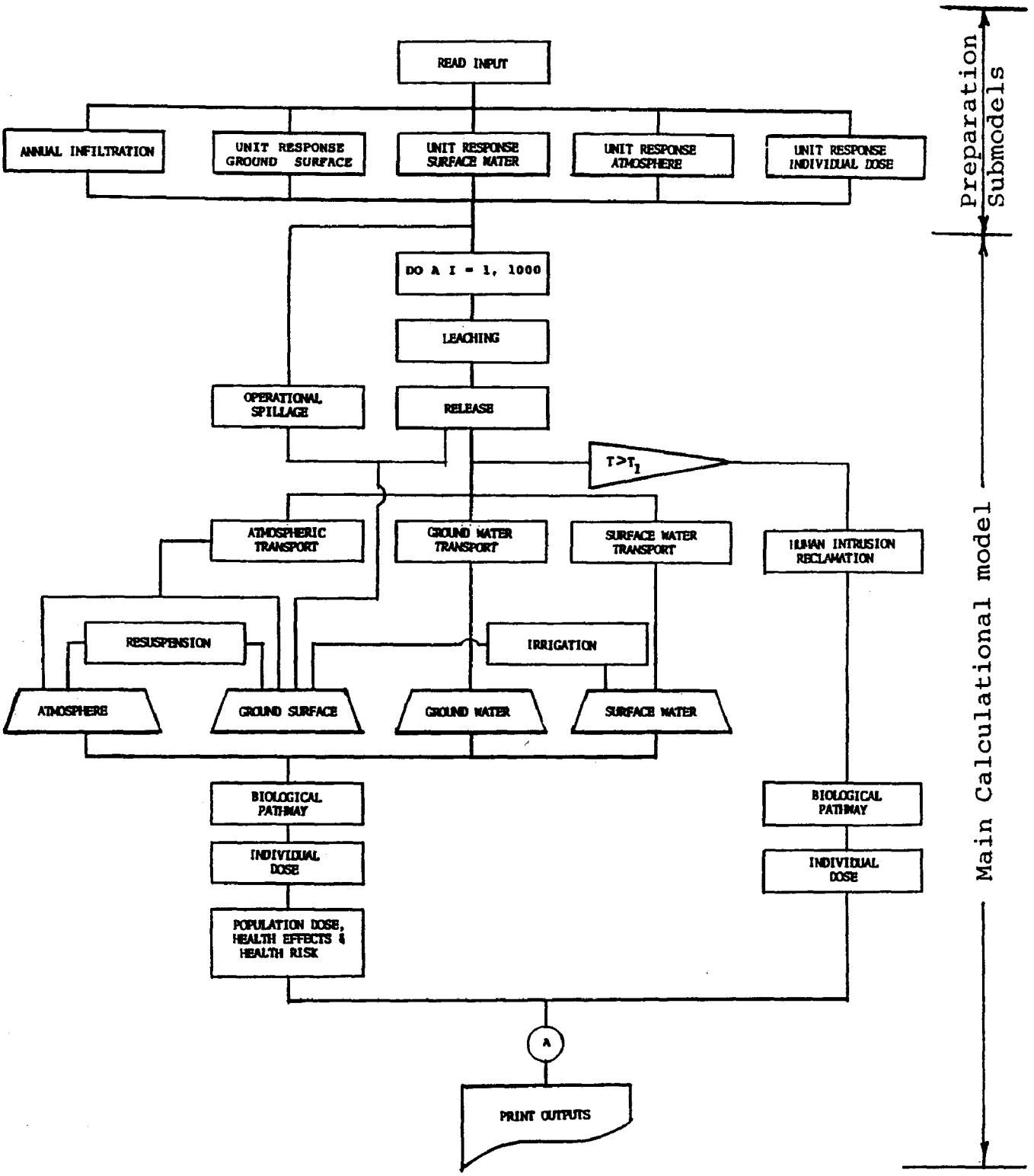

Figure 1. Block Diagram of EPA Environmental Assessment Model for the Shallow Land Disposal of LLW.

we took the following steps; we, (1) reviewed existing assessment models, (2) selected viable models from those reviewed, (3) utilized viable submodels from the models selected, and (4) filled in any gaps with new or improved submodels.

A recent review sponsored by ORNL identified over 350 codes or models that are available which might have application to LLW management and disposal.(14) More recently, R. W. Nelson identified more than one hundred groundwater models which might be useful for LLW management.(15) These reviews clearly point out the size of the task of reviewing "all available" models and of culling and selecting appropriate models and submodels. We selected the following models for in depth review:

- NRC model for waste classification (NRC-FBD)(16);
- NRC model for LLW EIS (NRC-D&M)(17);
- DOE model for SLD disposal site at Savannah River (DOE-SRL)(18)
- AIF SLD assessment model (AIF-D&M)(19);
- EPA model for assessing deep geological disposal of HLW (EPA-LOG)(20);
- EPA model for HLW standard (EPA-HLW)(21); and
- EPA models for Clean Air Act (EPA-CAA)(22).

We are continuing to review new models coming on the scene to take advantage of new and improved approaches. For example, the new NRC model for systems analysis of SLD (23) looks very promising and useful. It has several submodels which could be very useful to our SLD model when they are developed. However, the approach of NRC's systems is different than EPA's on several points. Also, it may not be completed in time for use in developing our standard. In any case, we tried not to duplicate the modeling efforts of others and, where possible, to use the best (for EPA's purposes) of others.

Findings of Model Review

From our review of the above models, we found that none of them met EPA's requirements without additions or modifications. We did find, however, that some existing submodels developed by EPA and others could be reasonable combined together without major modifications. The infiltration, leaching, release, and groundwater transport submodels were an exception. In some cases, EPA models and

submodels were available for adaption and EPA models were selected for the SLD model to maintain consistency with current EPA policies and calculational practices. Figure 2 summarizes the comparison of the risk assessment models which were reviewed in detail prior to design of EPA's LLW model. An estimate of the relative suitability of submodels within these models for use in EPA's risk assessment model for SLD are indicated. A description of key differences between EPA submodels and approaches and other assessment models follows.

Among the risk assessment models reviewed, the infiltration, leaching and release processes had been lumped together into a combined simple model represented by a leaching rate which is proportional to the remaining inventory of radionuclides. This is too simple for realistic health risk and benefit/cost assessments. Such a combined model assumes a constant leaching rate. This rate must be guessed at over an infinite period of time.

A significant problem with this type of model is that it can only be validated through extensive field and laboratory studies. It is doubtful that even this approach can successfully accomodate all of the boundary conditions and factors involved. For example, the leaching rate of radionuclides from the wastes is affected by many parameters such as trench cap conditons, the amount of infiltration, the accumulation of water in the trenches, waste form characteristics, and the properties of the radionuclides. Therefore, the reliability of estimates of leaching rates will be extremely variable, even if they can be determined with field data.

In addition, leaching and release represent two different processes. Predominant factors governing these processes include the rate of infiltration, accumulation of water in the trench, waste form, and disposal site characteristics. The processes may be controlled through changes in waste preparation and disposal operations such as trench engineering, waste pretreatment and site selection. Use of the existing combined models for reasonably accurate predictions at a site would require expensive and time consuming pilot studies before this type of model would have a valid application.

A more realistic yet simple way of modeling these processes is to subdivide them into three separate components, using dynamic simulation models for the infiltration, leaching and release processes. A major advantage of using individual dynamic simulation models for each of the processes is that it allows one to simulate changes in waste treatment and disposal procedures, which further allows an analysis of the costs and benefits of these changes. Another advantage is that the basic input parameters for these

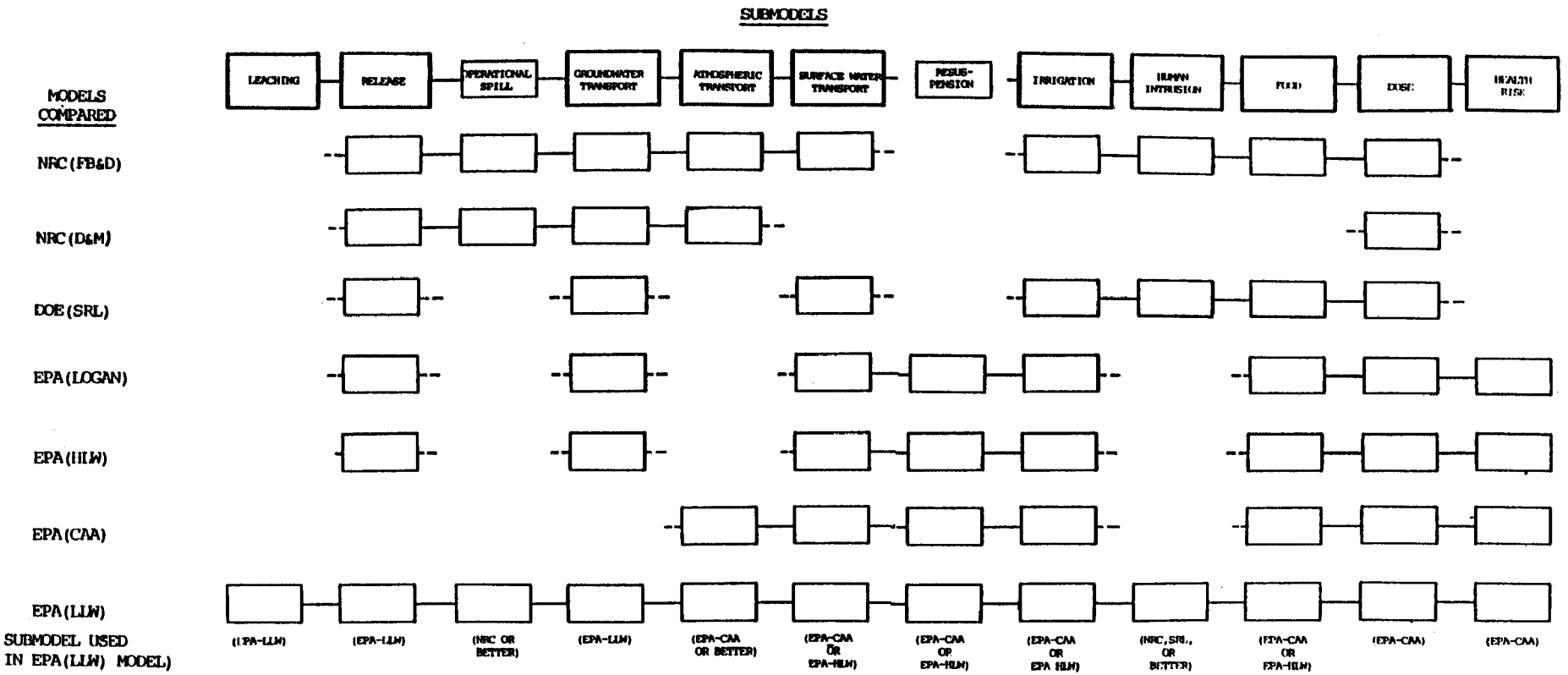

Figure 2. The availability of submodels from existing risk assessment models and those selected for use in the EPA risk assessment model.

dynamic models can be obtained from simple field measurements and laboratory tests without great delays or expense for lengthy field and laboratory studies.

Some of the groundwater transport which were models reviewed utilized an analytical approach which is economical to compute but is limited by a specific boundary condition. The boundary condition commonly used for these models, except the D&M model, is an exponentially depleted release rate. However, the output function of radionuclides released from a realistic physical model is normally an irregular function of time and may not reasonably be approximated by the above boundary condition. Therefore, those existing models which used an analytical approach, were not applicable to our needs.

The groundwater transport models, which used a numerical approach, are generally not economical to operate if the numerical error is to be controlled to an acceptable level. This is because improper division of time and space increments may introduce an unacceptable level of numerical error. Therefore, the numerical groundwater transport model is, in general, considered to be undesirable for use in a risk assessment model. In addition computational times and costs of numerical models are generally too high for risk assessment models where it intended to make a large number of calcualtions.

INFILTRATION, LEACHING AND RELEASE SUBMODELS

The release of radionuclides from the waste disposal trench to the geosphere is a complicated series of physical processes which includes infiltration, leaching and release from the trenches. The rate of infiltration of water through the trench cover is a function of meteorological conditions such as precipitation, temperature, wind speed and air humidity; the characteristics of the trench cover; and drainage conditions at the site. The leaching of radionuclides from the waste is a function of the form and sorption characteristics of the waste and the duration of its inundation in trench water. The rate of release of radionuclides from the trench is a function of the transmisivity of the host formation, its natural sorptive and retentive properties and the pressure head of water in the trench.

The basic system equations for each of these processes are briefly described in the following sections. It should be noted that the basic system equations presented herein cannot be directly employed as basic equations for risk assessment modeling applications because they are too sophisticated mathematically and will be simplified further during development of the EPA model.

Infiltration Submodel

The infiltration submodel is intended to simulate the average annual rate of infiltration through the trench cover during and subsequent to a period of precipitation. Figure 3 is a schematic diagram of the hydrological system associated with the earthen trench cover. It includes overland flow and subsurface flow systems. The momentum and continuity equations for each of these subsystems are

$$\frac{1}{g}\frac{\partial u}{\partial t} + \frac{u}{g}\frac{\partial u}{\partial x} + \frac{\partial h}{\partial x} - \sin\theta + \frac{n^2 u^2}{h^{4/3}} = 0 \qquad (1)$$

$$\frac{\partial h}{\partial t} + h\frac{\partial u}{\partial x} + u\frac{\partial h}{\partial x} = R(t) - E(t) - v(t) \qquad (2)$$

for the overland flow subsystem and

$$v = -K\frac{\partial(\Psi + y)}{\partial y} \qquad (3)$$

$$\frac{\partial s}{\partial t} = -\frac{\partial U}{\partial y} \qquad (4)$$

for the subsurface flow system. In the above equations, u and v are the velocities of water along and perpendicular to the slope of the trench cover, respectively; h is the depth of overland flow; D is the thickness of the trench cover; K is the permeability of the trench cover; n is the Manning coefficient of roughness of the surface of the trench cover; R is the rate of rainfall: E is the rate of evaporation; Ψ is the soil moisture tension potential of the trench cover; S is the water content of the trench cover: x and y are the coordinates along and perpendicular to the slope of the trench cover repectively; and t is the time.

Since the above system equations are extremely difficult to solve and our primary interest is determining the average infiltration rate v, one may simplify the momentum equation by neglecting the convective acceleration and local acceleration terms appearing in Equation 1. When this is done, Equation 1 can be simplified and it yields

$$q = \frac{H^{5/3}\sqrt{\sin\theta}}{n} \qquad (5)$$

and Equation 2, the continuity equation, can be rewritten as

$$\frac{dH}{dt} = R(t) - E(t) - v(t) - \frac{q}{L} \qquad (6)$$

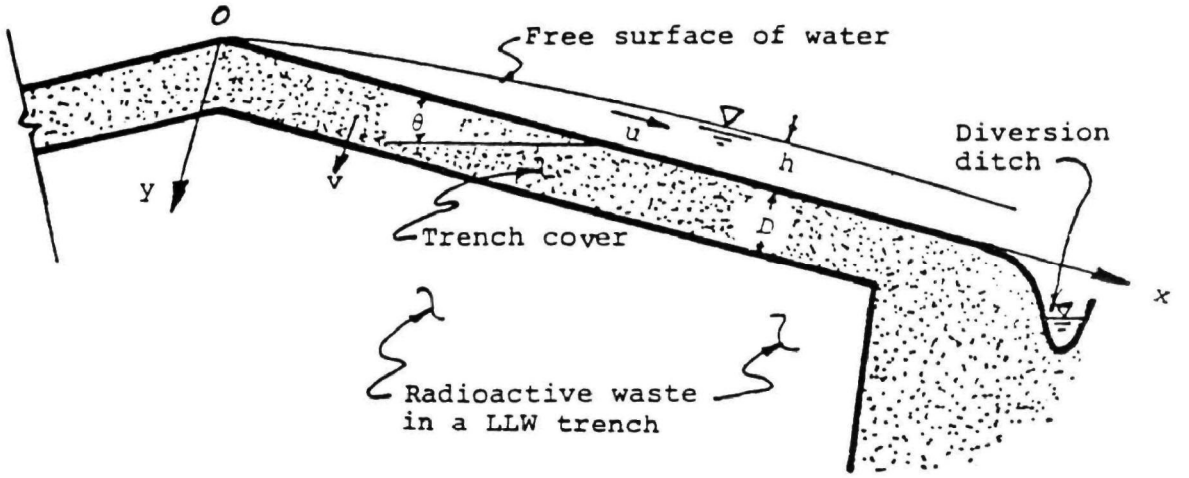

Figure 3. Schematic Drawing of a Two-Dimensional Infiltration Model for a LLW Burial Trench

where q is the overland flow and H is the average depth of flow.

Equations 5, 6, 3 and 4 are the basic equations for solving the infiltration of precipitation through the trench cover having overland runoff q, depth of overland flow H and the moisture content of the trench cover S as dependent variables. These system equations can be further simplified and solved by a linearized equation for a tank model.(24)

Leaching and Release Submodels

Some LLW, such as bulky solids and trash, are disposed of directly into the trench in their original form. Other LLW, which were originally liquids or slurries, are solidified to immobilize the radionuclides in suspension or solution before disposing of them into the trenches. EPA's risk assessment model is designed to simulate the leaching and release of both types of waste. The following discussion uses as its general case, a 55-gallon drum (or larger container) filled with solidified liquid waste such as evaporator concentrates solidified in cement and is applicable for the leaching and release of one radionuclide.

The basic mass balance equation governing the radionuclide concentration within the solidified liquid waste has been derived by Hung (13) as

$$\frac{\partial C_1}{\partial t} = \frac{D_e}{R\varepsilon}\frac{\partial^2 C_1}{\partial x^2} - \lambda_d C_1 \qquad (7)$$

where C_1 is the radionuclide concentration in the solidified waste; D_e is the effective dispersivity: R is the retardation factor; ε is the porosity: λ_d is the decay constant; x is a coordinate; and t is time. The initial conditions used to solve this equation are

$$\left.\begin{aligned} C_1 &= C_0, \quad \text{for } 0 \le x \le L \\ C_2 &= 0, \end{aligned}\right\} \qquad (8)$$

and the boundary conditions are

$$\left.\begin{aligned} C_1 &= C_2(t) \quad \text{at } x = 0 \\ \frac{dC_1}{dx} &= 0, \quad \text{at } x = L \end{aligned}\right\} \qquad (9)$$

In these equations, C_2 is the concentration of the radionuclide in the trench water: L is the leaching length, which is computed from the ratio of the volume of the waste container to its surface area; and C_o is the initial radionuclide concentration in the solidified waste.

The computations for solving Equation 7 for solidified wastes are too complicated to integrate into EPA's risk assessment model. It was determined, however, that the processes described by this submodel can further be approximated and simplified by eliminating the space independent variable. Thus Equation 7 can be simplified from a partial differential equation into an ordinary differential equation.

Despite the appearance of adding complexity to modeling the infiltration, leaching and release processes (i.e., going from a simple declining percentage model to three dynamic simulation models), in our opinion, it is a necessary step if the effects of changes and improvements in radionuclide retention due to waste solidification and engineering changes to the trench cap are to be evaluated. Further, such detailed analyses are necessary to provide data for our cost/benefit analyses to support our standard.

The dynamic equation for the exfiltration of water from the trench can be approximated by

$$\left.\begin{aligned} Q_e &= A_t K_h, && \text{for } H_w > 0 \\ Q_e &= 0, && \text{for } H_w \leq 0 \end{aligned}\right\} \qquad (10)$$

Where A_t is the bottom area of the trench; K_h is the hydraulic conductivity of the host formation; and H_w is the depth of water in trench. The rate of radionuclide release can thereafter be computed from the rate of water leaving the trench and the radionuclide concentration C_2 in the trench water.

The above basic equations consider the water which has been solidified to improve radionuclide retention in the waste. For wastes which were originally solid or are liquid, the diffusivity process is sufficiently large to maintain $C_1=C_2$ at all times. Therefore, computation of leaching and release for these types of waste is much simpler than for wastes which have been solidified.

GROUNDWATER TRANSPORT SUBMODEL

To date, more than one hundred and eight groundwater transport models have been developed.(15) However, some of these models fail

to consider the process of radioactive decay and/or sorption and are, therefore, not suitable for application to health effects evaluations. The rest of the models which may be suitable for health effects evaluation can be subdivided into two groups, the analytical model and the numerical model. In general, analytical models are limited by specific mathematical boundary conditions which require some approximation of actual physical conditions. As a result, these models suffer considerable error in simulation due to these approximations.

A numerical model requires, in general, many more computations than the analytical model does. In addition the accuracy of simulation depends greatly on the adjustments of time and space increments. Severe errors may result if they are not properly adjusted. On the other hand, obtaining proper adjustment of these increments may, in some cases, result in excessive computer time for making the simulation. Thus, calculational costs may become prohibitive when the model is applied to long-term simulations such as health effects evaluations.

For example, Hung (12) reviewed the use of a finite element model developed by Duguid and Reeves (25) to simulate the vertical migration of tritium from a burial trench towards the groundwater table at the West Valley (NY) disposal site.(26) This application required seven minutes of central computer process time on a UNIVAC-110 to simulate 200 years of real time. If it is further assumed that 1000 years of real time would be required to simulate the vertical migration of a radionuclide to the nearest underlying aquifer and its horizontal migration in the groundwater to the nearest discharge point, 700 minutes of processing time would be required for simulating ten radionuclides. This would be equivalant to $10,000 per run on a commercial computer, a cost which is unquestionably excessive when a number of runs may be required to test the effects of changing several parameters.

A one-dimensional numerical model developed for EPA by INTERA Environmental Consultants, Inc., (27) employs the finite difference method. In a review of this model, Hung (12) found that it had a computer processing cost of $200 for simulating the migration of a single radionuclide in an aquifer one mile long for a real time of 100,000 years. This, also, is too costly when many other radionuclides and pathways must be considered.

Several analytical models, for example those by Lester, Jansen, and Burkholder (28), Ford Bacon, and Davis, Utah, Inc. (16), and Dames and Moore (17), have made considerable contributions to groundwater transport modeling by simplifying the procedures for simulation. However, the application of these models to health

effects assessments is limited because it requires converting approximations of physical boundary conditions into mathematical forms which meet the requirements of an analytical model. This may result in considerable error in some cases.

For the reasons outlined above, the existing numerical and analytical models seemed either too costly to process or contained the possibility of introducing unexpected errors of analysis when applied to health risk calculations. A more economical and, we believe, more suitable groundwater transport model for health risk assessment has been developed by Hung.(12)

The basic equation for the groundwater transport model is expressed by

$$\dot{Q}(t) = \eta \mathrm{Exp}(-RL\lambda_d/V)\dot{Q}_0(t-RL/V) \qquad (11)$$

in which Q and Q_o are the rate of radionuclide release at the discharge end and at the trench; η is the correction factor for health effects; R is the retardation factor: L is the length of the aquifer; λ_d is the decay constant for the radionuclide; and V is the interstitial velocity of groundwater flow. Because this is an algebraic equation, it is simple and economical to process when integrated into a health effects assessment model.

The correction factor closely approximates and corrects for the effects of dispersion. The correction factor η was expressed as

$$\eta = \frac{\int_0^\infty (1/2)\sqrt{(RP/\pi\theta^3)}\,\mathrm{Exp}\{-N_d\theta-(P\theta/4R)(R/\theta-1)^2\}d\theta}{\mathrm{Exp}(-RL\lambda_d/V)} \qquad (12)$$

Derivation of η is described in detail in a separate paper by Hung.(12)

SUMMARY

EPA is developing an environmental assessment model to support its environmental standard for the management and disposal of LLW. This model will be used to analyze the potential transport and release of radionuclides to the biosphere and to estimate the

subsequent doses, health risks, and costs from disposing of LLW by shallow land disposal.

The SLD model is a generic, analytical systems model for analyzing a disposal facility as a complete "disposal system" which includes the waste, the site geology, hydrology and climate, and all of the pathways from it. It can be used for analyzing the performance of planned and existing disposal facilities, and is particularly suited to evaluating the effects of changes to a disposal facility (i.e., changes in waste form and packaging, trench cap design or water control engineering). The SLD model is sufficiently flexible to use for analyzing sites having disposal media with a wide range of permeabilities and located in either humid or arid climates.

Improvements have been made in EPA's SLD model for modeling the influx of water into the trenches, the leaching of radionuclides from the waste, and the release of radionuclides from the trenches. These features are particularly important for evaluating LLW management and disposal practices because they are the principle parts of the SLD disposal system which man can change to increase the retention capability of a disposal facility.

Individual dynamic simulation models have been developed for infiltration, leaching and release which can use information from simple laboratory tests and field measurements for input data. These separate submodels allow one to simulate changes in the performance of a disposal facility caused by changes in waste treatment and packaging, trench cover modification and site water control engineering. This further allows one to analyze the costs and benefits of any changes. The SLD model also has a new groundwater transport submodel which includes a correction factor for dispersivity, even though the model is an analytical, one-dimensional model. The basic transport equations for these four submodels are presented. These basic equations will be simplified further during coding of the model. The other submodels are, for the most part, being adapted from existing models with minor modifications.

It is believed that the basic features of EPA's SLD model, such as economical operation, realistic simulation, use of generally available data, and capability of evaluating changes to a disposal facility, will make it a potentially useful model for other government agencies and industry who are interested in assessing the impact of proposed or existing disposal facilities. When completed, coding and documentation on it will be made available to interested parties.

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RISK ASSESSMENT AND RADIOACTIVE WASTE MANAGEMENT*

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ABSTRACT

In order to evaluate the hazard of toxic material buried underground, the concept of geotoxicity is presented. This concept permits the development of a tool for quantifying the degree of hazard of such material, and this tool is formulated as the geotoxicity hazard index. The components of the geotoxicity hazard index are described and discussed. Finally, some sample results are offered. A more detailed description can be found in the report "A Hazard Index for Underground Toxic Material," UCRL-52889, June 1980.

INTRODUCTION

The waste management hazard assessment program at LLNL has as its objective the development and assessment of rationale for radioactive waste management programs. The bulk of previous research in waste management programs has been devoted to the development of methodologies for handling and disposing of waste. Our program deals with the development of rationale. We are more concerned with the "Why?", than the "How to" aspects of the problem. Obviously, predictive modeling plays an important role in this work. In this paper we will cover our overall program and in particular, our efforts in developing a hazard index for underground toxic material which can perhaps provide an alternative approach toward defining risks. A hazard index might also provide some insight for waste management programs in determining "how good is good enough."

GEOTOXICITY

The overall approach to problem definition which we apply is the geotoxicity study. This study involves the characterization and assessment of the harmful effects of hazardous material buried in the earth's

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*This work was performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore Laboratory under contract No. W-7405-Eng-48.

crust by either man or nature. It should be recognized that incorporation of toxic materials in the earths crust via radioactive or toxic waste burial does not present unique or unprecedented risks to health and the environment. Nature has done essentially the same throughout the entire history of the earth in toxic mineral deposits. The geotoxicity concept utilizes this perspective to provide useful insights on the fate of these materials in the biosphere. B. L. Cohen has characterized the approach as using the earth itself as a large analog computer. In any case, it is most useful to have a measure or "yardstick" with which one may characterize the hazard of toxic material buried underground. With this objective in mind we are developing the Geotoxicity Hazard Index (GHI). This index may be used:

- to provide an easy to use comparative tool
- to gain perspective on geotoxicity
- to enable screening of concepts for the disposal of toxic material
- to provide insight on the relative hazard of toxic components
- to permit examination of the source of toxic hazard

It should be noted that the GHI is not intended to substitute for detailed systems modeling used for prediction of specific consequences and their magnitude. It can however be used to provide additional insight on the severity of the general problem (or lack of it). Also, the results of systems analysis can provide valuable input to hazard index determinations.

REVIEW OF PREVIOUS WORK

The approach that was taken in our work was to review and evaluate previous efforts in the safety index area to either select an existing index, or identify the requirements for a new index if, as it turned out, a new index would be required.

Evaluation of previous work resulted in a classification of indices as shown on the first portion of SLIDE #1. The first category consists of the simple indices which are measures of quantity such as mass, number of curies, volume, heat output, and so on. Somewhat more complicated are the toxic indices which incorporate specific toxicity in addition to the quantity of material. Some examples of this second category are the dilution volume hazard index or the volume of water required in dilution to drinking water levels, and the number of lethal doses index. These indices are widely used in the literature. However, they are measures of toxicity and not hazard. Clearly, a material can be toxic but not particularly hazardous if there does not exist a means for exposure to the material. The next level of complexity involves indices which, in addition to toxicity, incorporate availability of the toxic material at the end of the transport process. Such indices may incorporate transport and radioactive decay effects. The final category consists of complex indices which include value judgement or decision analysis. This approach was rejected for the geotoxicity hazard index. The incorporation

Slide 1

Our Review of Previous Work Included:

- Evaluation of previous indices for radioactive and stable toxic materials
  - simple indices (mass, volume, heat, etc.)
  - toxic indices (toxicity and quantity)
  - complex indices (incorporating availability)
  - complex indices (including value judgment/decision theory)
- Determination of desirable features for our index
  - simple, easy to use
  - containing enough information to be meaningful
  - applicable to both radioactive and stable toxic materials
  - emplaced by man or nature
- Identification of factors that could be included

of value judgement greatly increases the level of subjectivity and therefore, such indices would be difficult to defend.

Since it was determined from our review that none of the previous indices met our objectives for a geotoxicity index, we used the review to focus on the desirable features and factors that could be included in the new index. The desirable features include simplicity in form to promote easy use, and, as a corresponding trade-off, sufficient complexity to provide for a meaningful measure of hazard. Other desired features are the capability to handle radioactive as well as stable toxic material, and natural deposition as well as emplacement by man.

There are several factors which could be included in an index of hazard. Some of these are shown on SLIDE #2. Of the parameters listed, the four on the left were considered basic requirements for our index; toxicity, availability, longevity or persistence, and transformation product effects are key parameters and have been explicitly incorporated into the Geotoxicity Hazard Index.

Chemical and physical form, and the effects of biological concentration are factors which are implicitly included in the previous four factors. Perceived harm as opposed to actual detriment could be included in an index, but, as stated earlier, this approach was rejected.

THE GEOTOXICITY HAZARD INDEX

Based upon the previously discussed considerations, a Geotoxicity Hazard Index (GHI) was developed in the following form.

$$GHI_i = TI_i \cdot P_i \cdot A_i \cdot C_i$$

$$GHI = \sum TI_i \cdot P_i \cdot A_i \cdot C_i$$

where

TI = toxicity index
P = persistence
A = availability
C = buildup correction
i = material index

For a given material i, GHI is determined as a product of four factors which represent toxicity, persistence, availability, and decay product buildup. The index can be viewed as a toxicity index which is modified by three dimensionless parameters to successively incorporate time, transport, and decay effects. For a mixture of toxic materials, the total GHI is obtained through summation of the individual indices for the toxic components. Each of the factors of the GHI will be discussed in turn.

Slide 2

POTENTIAL PARAMETERS FOR A HAZARD MEASURE INCLUDE:

- TOXICITY
- AVAILABILITY (TRANSPORT)
- LONGEVITY
- TRANSFORMATION PRODUCTS
- CHEMICAL FORM
- PHYSICAL FORM
- BIOACCUMULATION
- PERCEIVED HARM

Toxicity Index

The first term in GHI is the toxicity index, TI (SLIDE #3). The basic toxicity index which was chosen is the public drinking water dilution volume. For radionuclides, it is the volume of water required for dilution to MPC level, while for stable toxic materials, it is the analagous volume relative to the EPA drinking water standards, or DWS. Both apply to public drinking water supplies. This choice of a toxicity index permits the intercomparison of radioactive and nonradioactive materials. While not based on a rigorous equivalence of effects, the comparability of MPC and DWS has been studied previously and they are probably the best available measures of relative toxicity, for chronic, low level exposures. SLIDE #3 shows some examples of specific toxicity values for several materials. To produce a toxicity index, the specific toxicity values would be multiplied by the appropriate material inventory. It is interesting to note the values for I-129 versus elemental mercury. On a unit mass basis, these materials are of comparable toxicity.

Persistence

The second factor in the GHI is the persistence factor, P (SLIDE #4). For stable materials, the persistence factor has a value of one; indicative of maximum persistence. For materials which decay, P has a value less than one. Persistence is determined as the average fraction of the original material which is present in undecayed form, over a reference 300 year time frame. The lower part of this slide illustrates the relationship between P and half-life. Also shown on SLIDE #4 are some examples of materials with half-lives running from infinity down to the 24 day half-life of Th-234.

Availability

The third term in the GHI is the availability factor, A (SLIDE #5), that relates the ingestion of a material to its concentration in the earth's crust. The availability factor, A, is durther defined in terms of a modification factor, m, and A_0 which is the average availability of the natural analog of the material under consideration. A_0 is the ratio of the ingestion rate of material i to its crustal abundance, divided by the same ratio for naturally occurring radium-226. The modification factor, m, is intended to account for differences between the actual burial conditions and the average conditions for the natural analog. For example, if a material is significantly less available than its natural analog because of isolation barriers, siting, waste form, depth, or other condition, the m factor would be significantly less than one. For availability no better or worse than the average natural conditions, m would be given a value of one. Some examples of the natural availability factor for several elements are also shown SLIDE #5. Note that radium, by definition, has a value of one. Other elements are

Slide 3

$$GHI = TI \cdot P \cdot A \cdot C$$

TI = TOXICITY INDEX: A MEASURE OF INNATE TOXICITY

- FOR RADIONUCLIDES: TI = Q/MPC
- FOR STABLE MATERIALS: TI = M/DWS
- PERMITS INTERCOMPARISON OF RADIOACTIVE AND NONRADIOACTIVE MATERIALS
- EXAMPLES:

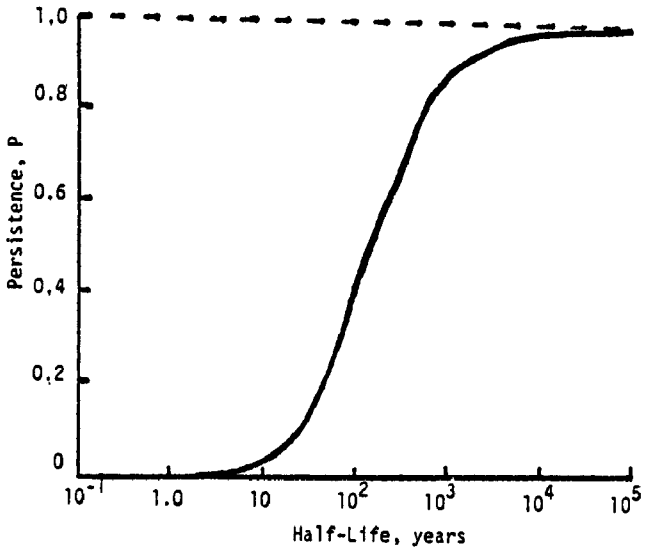
MATERIAL	SPECIFIC TOXICITY (per Curie)	SPECIFIC TOXICITY (per gram)
SR-90	10^7 m^3 per Curie	1.4×10^9 m^3 per gram
PU-239	2×10^5 m^3 per Curie	1.2×10^4 m^3 per gram
H-3	3×10^2 m^3 per Curie	2.9×10^6 m^3 per gram
I-129	2.5×10^6 m^3 per Curie	4.4×10^2 m^3 per gram
MERCURY	---	5.0×10^2 m^3 per gram
LEAD	---	2.0×10^1 m^3 per gram

Slide 4

$$GHI = TI \cdot P \cdot A \cdot C$$

P = PERSISTENCE FACTOR

- FOR STABLE MATERIALS, P = 1.0
- FOR DECAYING MATERIALS, $P \leq 1.0$
- PERSISTENCE IS JUDGED RELATIVE TO A 300 YEAR TIME PERIOD



EXAMPLES:

MATERIAL	HALF-LIFE	P
STABLE LEAD	∞	1.0
U - 238	4.5×10^9	1.0
PU - 238	88 YEARS	.38
SR - 90	28 YEARS	.14
TH - 234	24 DAYS	3.2×10^{-4}

Slide 5

$$GHI = TI \cdot P \cdot A \cdot C$$

A = AVAILABILITY FACTOR

- A IS THE FACTOR THAT RELATES THE INGESTION RATE OF A MATERIAL TO ITS CONCENTRATION IN THE EARTH'S CRUST
- $A = m\,A_0$, WHERE $A_0 = \dfrac{\text{INGESTION RATE}_i \;/\; \text{CRUSTAL ABUNDANCE}_i}{\text{INGESTION RATE}_{Ra} \;/\; \text{CRUSTAL ABUNDANCE}_{Ra}}$
  - A_0 IS THE AVAILABILITY OF THE NATURAL ANALOG
  - m IS A MODIFICATION FACTOR THAT ACCOUNTS FOR DIFFERENCES BETWEEN ACTUAL BURIAL CONDITIONS AND THE NATURAL ANALOG
  - EXAMPLES:

ELEMENT	A_0
RADIUM	1.0
LEAD	9.7
URANIUM	.27
IODINE	54.8

either more or less available in nature than radium, and these differences are reflected in their values for A_0.

Buildup Correction

The last component of GHI is C, the buildup correction factor (SLIDE #6). This factor is used to accommodate the buildup of decay progeny more toxic than the parent. Two examples are the decay of U-238 through Ra-226 to stable lead, and the transformation of elemental mercury into the more toxic methylated form. SLIDE #6 shows graphically how C is determined. On the right side of SLIDE #6 is a table which gives some examples of the buildup correction factors for several materials. It should be noted that in the majority of cases, C is equal to one. Materials with a significant buildup of decay toxicity are the exception rather than the rule. U-238 is the most extreme case which we have identified.

SAMPLE RESULTS

In order to demonstrate the use of the Geotoxicity Hazard Index, several representative toxic material deposits were considered. SLIDE #7 shows the results of the GHI calculations for these sample cases. While they involve several assumptions and simplifications, they are shown to illustrate the nature of the calculational results and to indicate the types of applications for which the GHI could be used. Future effort on the GHI will include converting the index into dimensionless form, and normalization to avoid the large powers of ten seen in these results.

Another goal toward which future effort will be devoted is improvement in estimation of the availability factor (A). This work is seen as an iterative process by incorporating new information into improved estimates. Further refinement of the calculational parameters will provide increased confidence in the results.

DISCLAIMER

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

Slide 6

$GHI = TI \cdot P \cdot A \cdot C$

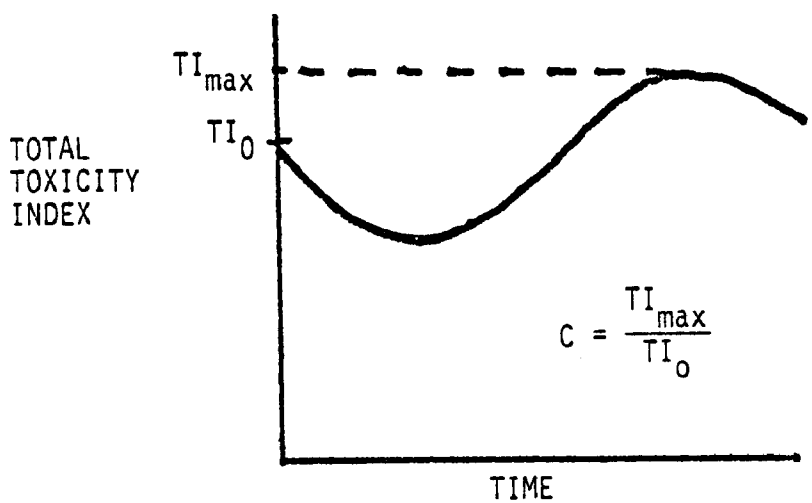
C = BUILDUP CORRECTION FACTOR

- C IS THE CORRECTION FACTOR TO ACCOUNT FOR THE BUILDUP OF DECAY PROGENY MORE TOXIC THAN THE PARENT

$$U^{238} \longrightarrow \cdots \longrightarrow RA^{226} \longrightarrow \cdots \longrightarrow PB^{206}$$

$$HG \longrightarrow HG\,(CH_3)_2$$

- EXAMPLES:



MATERIAL	C
U - 238	4.5×10^3
NP - 237	79
PU - 239	1.0
ARSENIC	1.0
LEAD	1.0

Slide 7

Results of Sample GHI Applications

Site	GHI
Low Level Waste Facility	2.7×10^{11}
High Level Waste Repository	4.4×10^{13}
Uranium Ore Deposit	3.0×10^{12}
Mercury Ore Deposit	1.3×10^{13}
Lead Ore Deposit	9.7×10^{12}

MODELING IN THE DETERMINATION OF USE CONDITIONS FOR A DECOMMISSIONED SHALLOW-LAND BURIAL SITE

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ABSTRACT

Because site stabilization results in smaller dollar costs and lower occupational doses than does waste removal, it is the preferred alternative for the decommissioning of shallow-land burial grounds. Release of a burial ground for public use following site stabilization would probably be on a conditional-use basis. A pathway modeling methodology has been developed for the evaluation of use conditions for a decommissioned site. The methodology consists of estimating the maximum annual dose to the maximum-exposed individual resulting from a specific use scenario. The methodology is sensitive to site parameters, to radionuclide inventories, and to uncertainties that exist in nuclide transport models and in the parameters used in the models to represent specific sites. Several research needs are identified that would result in improved predictions of radionuclide migration from shallow-land burial grounds.

INTRODUCTION

A study,[1] sponsored by the Nuclear Regulatory Commission, was performed to estimate dollar costs and public and occupational radiation doses resulting from decommissioning reference shallow-land burial grounds by the decommissioning alternatives of 1) site stabilization plus long-term care and 2) waste removal. On the basis of minimum cost and occupational radiation dose, site stabilization is the preferred decommissioning alternative.

Site stabilization implies that all or some portion of the waste is left in place, and release of the site would probably be on a conditional-use basis. A methodology was developed for evaluating scenarios for the conditional or unrestricted release of a burial ground after burial operations cease. The methodology uses pathway modeling techniques to estimate the maximum annual dose to the maximum-exposed individual for various site use scenarios. The maximum annual doses for the given use scenarios are compared to determine which scenario is more appropriate.

Results and conclusions derived from this pathway analysis approach depend on the site characteristics, on the burial ground radionuclide inventory, on the mathematical models used to evaluate potential exposure pathways and estimate radiation doses, and on the parameters used in the models. Uncertainties exist in the models used to estimate radionuclide

transport and in the parameters and boundary conditions used in the models to represent specific sites. These uncertainties can affect the validity and seriously limit the usefulness of the pathway methodology approach.

DECOMMISSIONING ALTERNATIVES

Decommissioning is defined as the measures taken at the end of a facility's operating life to ensure that future risk to public safety from the facility is within acceptable bounds. For a shallow-land burial site, the basic decommissioning alternatives are 1) site stabilization followed by a period of long-term care and 2) waste removal.

Site stabilization involves the use of engineered procedures to reduce the rate and extent of radionuclide migration from buried wastes left in place in a decommissioned shallow-land burial ground. Potential site stabilization activities include:

- engineered routing/flow control of ground and surface water
- modification of trench caps to minimize water infiltration into the trenches
- stabilization of the land surface and erosion control
- grouting and/or use of chemical additives to reduce the mobility of the waste
- control of plants and animals that might disrupt surface stabilization measures or transport radioactivity from the trenches
- erection of physical barriers to control human activities at the site.

Site stabilization implies that all or some portion of the waste is left in place, and onsite public activities are restricted to land uses that do not result in excessive public exposure to radiation and that do not compromise stabilization procedures or waste confinement.

Site stabilization is followed by a period of long-term care of the site. Long-term care activities include site surveillance and maintenance, environmental monitoring, and administrative procedures for control of the site. Long-term care continues until it is determined that the radioactivity at the site has decayed to the point where the waste no longer poses a significant radiological hazard, or until additional actions are taken to reach this point.

Waste removal involves the exhumation of buried waste and contaminated soil, packaging of the waste and soil, transportation, and reburial of the waste at another disposal site. Because of the potential for significant radiation dose to decommissioning workers and the high dollar costs, waste

removal would likely be considered only in situations where site stabilization and long-term care are insufficient to ensure the continued capability of the site to provide adequate containment of the buried waste.

At a particular site, combinations of decommissioning activities may be necessary to ensure that future risk from buried radioactive material is within acceptable bounds. Combinations of decommissioning alternatives may be necessary when individual burial trenches are known to contain high concentrations of transuranic waste or waste mixed with organic complexing agents. In these instances, the removal of the waste from part or all of a particular trench or trenches may be a requirement in conjunction with stabilization of the rest of the site. Partial waste relocation may also be required if burial trenches are located in an area with geologic or hydrologic characteristics that make stabilization a costly or technically unfeasible alternative. In this case, the waste removed from one trench might be reburied in another onsite trench or it might be transported to another disposal site.

DECOMMISSIONING OF REFERENCE SITES

Two generic burial grounds, one located on an arid western site and the other located on a humid eastern site, were used as reference facilities. The two burial grounds were assumed to have the same site capacity for waste, the same radioactive waste inventory, and similar trench characteristics and operating procedures. The climate, geology, and hydrology of the two sites were chosen to be typical of actual western and eastern sites. Each site description provided a basis for evaluating decommissioning methods and costs, and for estimating possible environmental impacts.

Costs of stabilization of the reference sites were estimated to range from $0.5 million to $8 million depending on the site and on the stabilization option chosen. Annual long-term care costs were estimated to range from $80,000 to $400,000.

Stabilization of a burial ground involves modification of and addition to surface soils, but no intentional uncovering or exhumation of buried waste. There is no transportation of radioactive waste. Therefore, routine site stabilization operations are not expected to result in any significant radiation dose to the general population. Modest exposure of decommissioning workers is expected; however, the dose rates would be less than those experienced during waste burial operations.

Waste removal was estimated to cost about $1.4 billion and to require approximately 1000 man-years of effort extending over a period of more than 20 years. Approximately 93% of the cost of waste removal was found to be associated with the packaging, shipment, and offsite disposal of the exhumed waste.

The 50-year committed dose equivalent to the affected population from routine waste removal operations was estimated to be very small compared to

the 50-year dose from natural background radiation. However, the occupational dose from waste removal was estimated to be approximately 30,000 man-rem, indicating that this decommissioning alternative can be very costly in terms of worker exposure to radiation.

ANALYSIS OF RELEASE CONDITIONS

Waste removal implies the complete removal of the buried waste and contaminated soil and can result in release of the site for unrestricted public use. Site stabilization implies that all or some portion of the buried waste is left in place. Release of a stabilized site would presumably be on a conditional-use basis, with public activities restricted to those that limit exposure to radiation and that do not compromise stabilization procedures or waste confinement. An important factor in determining the appropriate decommissioning alternative for a particular site is the estimated risk to the public from the decommissioned site.

A methodology was developed for predicting conditions for the conditional or unrestricted release of a burial ground after burial operations cease. The methodology consists of estimating the calculated maximum annual dose to the maximum-exposed individual resulting from a specific release scenario. The maximum annual doses from different scenarios are compared to determine which scenario is more appropriate. Doses to the maximum-exposed individual are calculated for all important exposure pathways using state-of-the-art modeling techniques. For the western site the important pathways are inhalation, direct external exposure, and ingestion of foods grown on the released decommissioned burial ground. For the eastern site, additional exposure pathways of importance are ingestion of aquatic foods from a nearby river and ingestion of water from a well drilled into an aquifer beneath the site.

Land-use scenarios are evaluated to determine release conditions following stabilization of the reference burial grounds. Examples of pathway analysis results are shown in Table 1. The dose numbers in the table are calculated maximum annual total body doses to an individual who lives and works on a conditionally released burial site having various use restrictions.

The first two values in the table are estimated maximum annual total body doses at the western and eastern sites during the first 50 years after site release assuming that individuals living on a site do not engage in excavation or drink water from onsite wells. The major contributors to dose are ^{63}Ni (assumed to be present in reactor decommissioning waste buried on the site) and ^{210}Pb (a radioactive daughter of ^{226}Ra). The third value is the estimated maximum annual total body dose at the western site assuming that excavation is permitted. Most of the dose from site excavation is from external exposure to the gamma radiation from ^{137}Cs.

TABLE 1. Maximum Annual Total Body Doses for Conditional Release of the Reference Burial Grounds With Different Use Restrictions(a)

Release Scenario	Maximum Annual Total Body Dose (mrem)
No excavation and no drinking of water from onsite wells - Western Site	4
No excavation and no drinking of water from onsite wells - Eastern Site	23
Excavation permitted - Western Site	380
Total erosion of trench overburden(b) - Western Site	1 300
Drinking permitted from contaminated well - Eastern Site	120 000

(a) Conditional release assumed to occur 200 years after site closure.
(b) Calculated at 450 years after site release (650 years after site closure).

The fourth value in the table is the estimated maximum annual total body dose at the western site assuming total erosion of the trench overburden. Total erosion is estimated to occur approximately 450 years after site release, based on the assumed erosion rate at the western site. Radionuclides that contribute most of the dose are ^{230}Th, ^{226}Ra, ^{210}Pb, ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu and ^{241}Am. While it is unlikely that site conditions would result in total overburden removal, this scenario demonstrates the importance of maintaining an adequate layer of overburden to prevent both crop root penetration into the waste and radionuclide dispersal by human activities or wind action. Institutional controls may be necessary to restrict human activities at a conditionally released site and to maintain an adequate depth of overburden.

The last value in the table is the estimated maximum annual total body dose at the eastern site assuming that the site resident obtains all of his drinking water from a shallow well drilled into the contaminated aquifer beneath the site. The dominant radionuclides contributing to the large annual dose are ^{14}C, ^{63}Ni, ^{90}Sr, ^{137}Cs, and ^{226}Ra.

For the reference burial sites, the pathway modeling approach indicates some restrictions that should be placed on a conditionally released site. Conditional release of the western site following site stabilization would be possible provided that the following actions are enforced:

- stabilize the ground surface to minimize surface erosion
- control the type of farming or other land use to prevent the growth of deep-rooted plants
- restrict activities that result in excavation of the site.

The conditional release of the decommissioned eastern site would include enforcement of the restrictions described for the western site, plus the following additional restrictions:

- prohibit the use of water from shallow wells drilled on or near the site
- maintain site drainage features to control surface water runoff and to prevent inundation of burial trenches with water
- stabilize the waste to minimize leaching to the aquifer, or control the use of aquatic organisms and water from nearby streams.

For the site stabilization alternative, unconditional release of the reference sites, even after a long-term care period of 200 years, would not be feasible because of the significant inventory of long-lived radionuclides in the buried waste.

The methodology developed for defining site use conditions is both site- and inventory-specific. The use restrictions listed above for the reference sites are given only as examples of results to be expected from the application of the modeling technique. The methodology must be reapplied and the radiation doses recalculated for each burial ground having a different radionuclide inventory and different site characteristics.

In addition to a dependence on site characteristics and radionuclide inventories, the results and conclusions of the pathway-modeling approach depend on the mathematical models used and on the parameters and boundary conditions employed with the models to represent specific site characteristics. Many uncertainties exist in the radionuclide transport models and in the parameters (e.g., distribution coefficients, dispersion coefficients, leach rates) used with the models. Because of these uncertainties, a generally conservative approach was attempted that may result in conservative (high) estimates of doses to the maximum-exposed individual.

TRANSPORT MODEL UNCERTAINTIES

Radionuclide migration via the groundwater pathway was simulated by use of the MMT (Multicomponent Mass Transport) model.[2] There are no established models for treating overland flow. To account for overland flow, the conservative approach is taken that the burial trenches are saturated with water. All of the water flowing through the trenches arrives at the surface and flows overland to the nearby river. No significant sorption is assumed during overland flow. These factors result in a conservatively high estimate of the radioactivity leached to the river by this pathway.

Although there are some uncertainties in nuclide transport models, the major uncertainties are in the parameters and boundary conditions fed into the models to represent specific sites. Order of magnitude uncertainties exist in values for soil permeability, dispersion coefficients, distribution coefficients (K_d), and leach rates. Some of these parameter values (e.g., Kd's and leach rates) are relatively easy to measure in the laboratory, but extremely difficult to measure under field conditions.

Because of the great difficulty of direct field measurement of Kd, values determined by laboratory measurement are normally used to calculate water transport of radionuclides. However, the validity of applying laboratory values to field situations is questionable because of the strong dependence of measured values of K_d on the physical and chemical conditions of measurement. Variables such as mineralogy, particle size, nature of solution, and chemical nature of the radioactive species can strongly affect the measured values. Table 2 gives examples of published values of K_d used in several studies of radionuclide migration. It is apparent that, for some radionuclides, significant differences exist between values reported by different authors.

Leach rates are influenced by many factors, including the characteristics of the radionuclide and of the waste material, the properties of the leachant, frequency of leachant changing, leaching time, and temperature. Specific field data on the leachability of radionuclides from waste buried in shallow-land burial sites are not available. The effects of chelates on the mobility of the radionuclides in buried waste are just beginning to be studied. Published leach-rate data come mainly from laboratory measurements in which small samples are leached by distilled water or by actual or simulated disposal-environment water. Laboratory leach-rate data are summarized in a recent Brookhaven National Laboratory report.[3] This report gives leach-rate values for cement monoliths that range from 10^{-1} to 10^{-9} g/cm^2-day.

An example of the effect of a change in leach rate on radionuclide concentration in a surface stream located 1 km from the reference eastern burial ground is shown in Figure 1 for a long-lived radionuclide with a small K_d value. The nuclide chosen is ^{99}Tc (K_d = 0). Increasing the assumed leach time* by an order of magnitude results in almost an order of magnitude decrease in the maximum radionuclide concentration in the ground water at the point

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* The leach time is the time required for the radioactive material to migrate from the burial ground at a constant leach rate.

TABLE 2. Reported Values of Distribution Coefficients for Selected Elements

Element	K_d (ℓ/kg) ARHCO[a]	NECO May[b]	NECO June[c]	Dames & Moore[d]	Leddicotte[e] Dry Site	Leddicotte[e] Humid Site	Staley[f] Sand	Staley[f] Silt & Clay
Co		138-593	700-800	75	1000	2500	100	1000
Sr	5-38	3-17	3-6	20	10	50	2	20
I				0	5	25	0.1	1
Cs	12-200	4000-9000	27-50	200	1000	2500	20	200
Pu	200			2000	1000	2500	200	2000
Am	1200			2000	1000	2500	70	700

(a) R. C. Arnett, D. J. Brown and R. G. Baca, Hanford Groundwater Transport Estimates for Hypothetical Radioactive Waste Incidents, ARH-LD-162, Atlantic Richfield Hanford Company, Richland, Washington, June 1977.

(b) Sheffield, Low-Level Radioactive Waste Disposal Site - Report of Additional Investigations Conducted During February and March, 1978, Nuclear Engineering Company, Inc. Louisville, Kentucky, Revised May 5, 1978. (Distribution coefficients for sands.)

(c) Sheffield, Illinois Low-Level Radioactive Waste Disposal Site - Responses to Questions, Nuclear Engineering Company, Inc., Washington, DC, June 29, 1978. (Distribution coefficients for loess, till, and shale.)

(d) A. E. Aikens, Jr., R. E. Berlin, J. Clancy and O. I. Oztunali, Generic Methodology for Assessment of Radiation Doses from Groundwater Migration of Radionuclides in LWR Wastes in Shallow-Land Burial Trenches, AIF/NESP-013, Prepared by Dames and Moore for Atomic Industrial Forum, Inc., January 1979. (Estimated values for a typical desert soil.)

(e) G. W. Leddicotte and W. A. Rodger, "Suggested Quantity and Concentration Limits to be Applied to Key Isotopes in Shallow Land Burial," in M. W. Carter, et al., Management of Low-Level Radioactive Waste, Vol. 2, New York, Pergamon Press, 1979.

(f) G. B. Staley, G. P. Turi and D. L. Schreiber, "Radionuclide Migration from Low-Level Waste: A Generic Overview," in M. W. Carter, et al., Management of Low-Level Radioactive Waste, Vol. 2, New York, Pergamon Press, 1979. (Distribution coefficients for sand were selected to be near the low end of the range of values reported in NUREG-0140. K_d values were increased by a factor of 10 for slit, clay, loess, and till.)

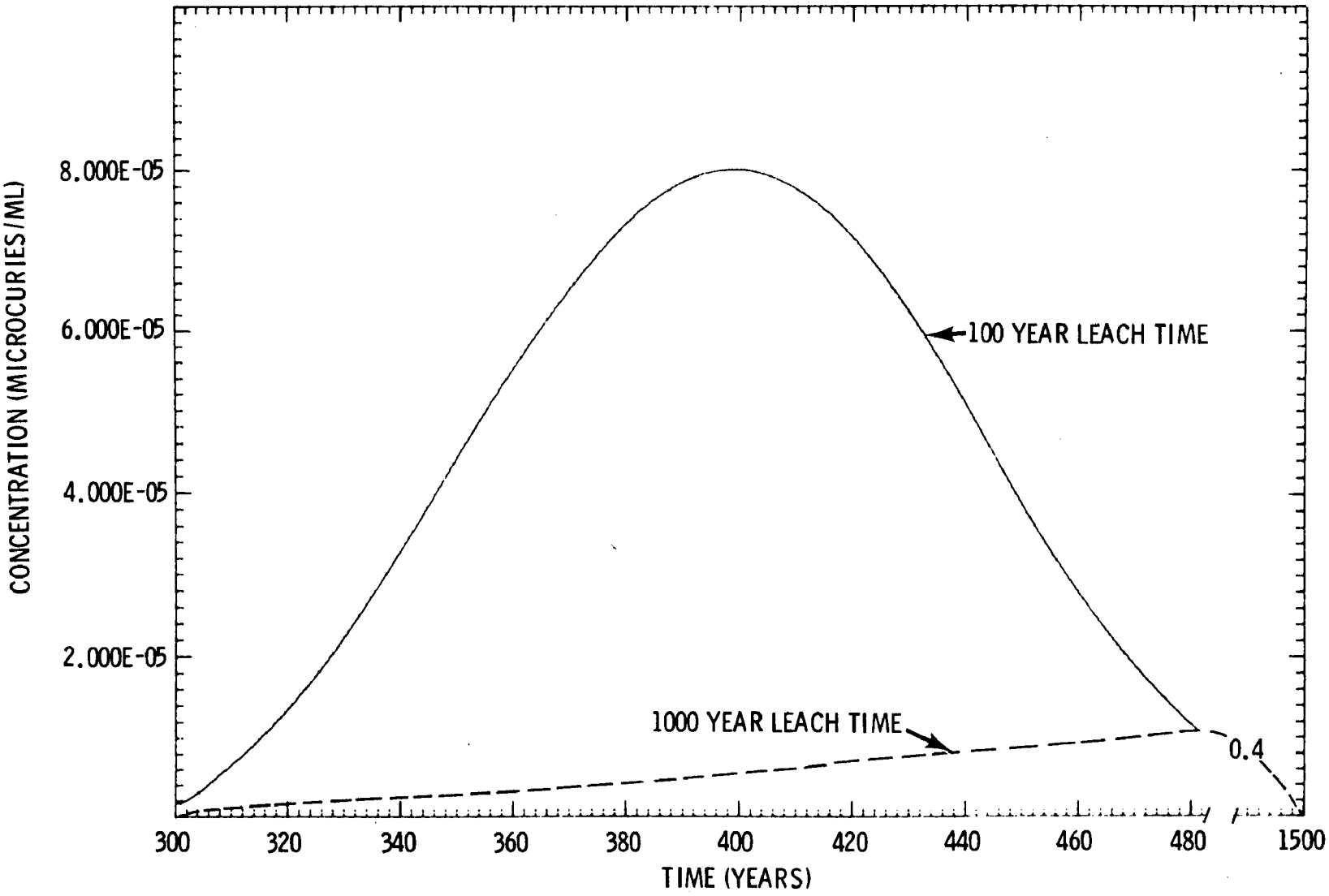

FIGURE 1. Predicted Technetium-99 Concentration in the Ground Water at the Point of Discharge to the Surface Stream

of discharge to the surface stream. It also results in a significant postponement of the time when this concentration attains its maximum value. For a radionuclide with a large K_d value, such as ^{230}Th, neither the maximum radionuclide concentration nor the time when the concentration attains its maximum value are significantly affected by an order of magnitude increase in leach time.

To improve the reliability of modeling studies of radionuclide transport, the need exists to demonstrate (verify) models on actual field sites and to develop better methods for measuring critical parameters such as distribution coefficients and leach rates under actual field conditions.

CONCLUSIONS

Decommissioning of reference shallow-land burial grounds by the alternative of waste removal is estimated to be much more expensive and to result in a much larger dose to decommissioning workers than site stabilization. Therefore, site stabilization is assumed to be the preferred decommissioning alternative. Site stabilization would probably result in the conditional release of a decommissioned site with use restrictions that would prevent excessive public exposure to radiation and that would ensure the adequate confinement of the buried waste.

A methodology has been developed for evaluating use restrictions for the conditional use of a burial ground after burial operations cease. The methodology uses pathway modeling techniques to estimate the calculated maximum annual dose to the maximum-exposed individual. Results and conclusions of the pathway modeling approach depend on the site characteristics, on the radionuclide inventories, and on the mathematical models and the parameters employed with the models to represent specific site characteristics.

Some uncertainties exist in nuclide transport models and major uncertainties exist in parameters and boundary conditions used in the models to represent a specific site. Several research needs can be identified that would result in improved predictions of radionuclide migration from shallow-land burial grounds. These research needs include:

1. development of transport models for overland flow
2. verification of models by comparison of predicted results with experimental results for real sites
3. identification and quantification of differences between field- and laboratory-measured values of distribution coefficients
4. determination of leach rates for specific radionuclides under field conditions
5. quantification of the effect of complexing agents on the mobility and transport of radionuclides from shallow-land burial grounds.

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A SYSTEMS MODEL FOR EVALUATING POPULATION DOSE FROM LOW-LEVEL WASTE ACTIVITIES

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ABSTRACT

This paper briefly describes a computer code developed to evaluate population dose or maximum individual dose from the various activities associated with shallow land burial of low-level wastes. The code, called BURYIT, treats a wide variety of scenarios to determine the effects of various parameters associated with siting, packaging and burial procedures on potential public exposure. In the analysis of radionuclide dispersal, BURYIT treats unsaturated zone seepage, aquifer transport, wind erosion and atmospheric transport. Population exposure pathways considered include direct exposure to undispersed wastes, direct exposure to contaminated air, direct exposure to contaminated ground, inhalation of contaminated air, and ingestion of contaminated food, water and milk.

INTRODUCTION

As part of an effort to develop analysis tools to support rulemaking and evaluation of license alternatives, the Nuclear Regulatory Commission* has sponsored the development of a systems level computer code (BURYIT) for use in assessing potential population dose from the various activities associated with low-level waste disposal. This code is currently under development by Science Applications, Inc. (SAI). When completed, it will derive either population dose or maximum individual dose for a wide variety of shallow land burial problems and conditions and will be used to evaluate the effects of several parameters including site location, site design, package integrity and operational procedures.

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*NMSS, Low-Level Waste Branch, J. D. Thomas, Project Officer.

PROBLEM DESCRIPTION

The problems which must be analyzed are varied and broad in scope. Many different release scenarios, ranging from short term to long term and involving different pathways, must be analyzed.

The scope of the problems was established early in the code development project. At that time, we visited five shallow-land burial sites (Maxey Flats, Barnwell, Richland (NECO), Hanford (DOE) and Beatty) and reviewed available literature to determine the nature of low-level wastes, their sources, and the most likely pathways which would lead to public exposure. We identified over fifty release scenarios for the various phases of low-level waste disposal. These scenarios ranged widely in characteristics and indicated the need for a very versatile code. For example, we wanted to be able to evaluate direct radiation exposure from wastes in transport or in an open pit, population exposure from contamination released by explosion or fire, and long-term exposure from nuclides leached from the site over periods of thousands of years.

CODE DESCRIPTION

Our approach to solving the variety of release scenarios was to develop a modular code which is software linked within the executive. This software linking enables BURYIT to call the appropriate analysis modules in the proper order for the particular scenario. For example, for a scenario involving leaching of nuclides to the surface followed by wind erosion and atmospheric transport, the scenario-related input data includes a specification for successive calls to the transport module for unsaturated soil, the wind erosion module, the air transport module and the dose evaluation module.

The executive, in solving a problem, may call some or all of the following modules:

PREDOS - This module loads required data for the nuclides to be analyzed. These data include half lives, dose factors, and transfer coefficients (for example, from grass to milk via cow). The data are extracted by direct access reads from a disk file containing data for about 350 radionuclides.

UNSAT - This module, which was derived from the HYDRO code, calculates the transport of radionuclides in the unsaturated soil zone. Given an isotope distribution in layered soil of specified characteristics, it calculates the nuclide distribution as a function of time, treating nuclide discharge to an aquifer and surfacing by evapotranspiration. The HYDRO code, from which UNSAT was derived, was developed in 1979 by SAI[1] based on an irrigation control model developed for the U.S. Environmental Protection Agency.[2]

AQUIFR - This module, which was developed from the PNL GETOUT code,[3] calculates nuclide transport in the saturated soil zone. An aquifer is treated as an one-dimensional flowing body with axial dispersion, sorption in the soil, and nuclide decay. The calculated output is the aquifer discharge rate for each radionuclide.

EROSIO - The EROSIO module calculates the rate at which soil is eroded by wind action. When the soil is contaminated, perhaps by a combination of leaching with evapotranspiration, EROSIO provides the quantity of radioisotopes released for atmospheric transport. EROSIO is a modification of the U.S. Department of Agriculture WEROS (wind erosion) code.[4]

ATMOS - The ATMOS module calculates the atmospheric transport of contaminants by use of standard Gaussian plume techniques. For the calculation of population dose, sector averaged air and ground radionuclide concentrations are calculated. Annual average results can be calculated based on an array of input weather conditions or results can be calculated for a specified input weather condition. Both wet and dry deposition and plume depletion are taken into account.

DOSE - This module calculates the maximum individual dose and population dose for the following exposure pathways: (a) direct exposure to an airborne cloud of contamination, (b) direct exposure from ground contamination, (c) inhalation of airborne contamination and (d) ingestion of contamination. The inhalation pathway includes resuspended contamination as well as nuclides in the initial plume. The ingestion pathway includes water via contaminated aquifer, leafy vegetables contaminated by atmospheric deposition, produce contaminated by root uptake, and beef and milk contaminated by animal ingestion of contaminated pasture grass.

For the maximum individual dose, the food and milk ingestion are based on quantities specified by NRC Regulatory Guide 1.109. For calculation of the population dose, it is assumed that all foods produced are eaten and thus contribute to population exposure. This production based (rather than consumption based) ingestion model eliminates the need for concern about foods exported from or imported into the analysis area.

DIRECT - This subroutine uses formulas from Rockwell[5] and Foderaro[6] to calculate the direct gamma radiation exposure from undispersed wastes. Example problems are direct radiation from wastes in the open pit or shielded or unshielded individual waste packages during transportation or processing.

DATA BASES

BURYIT extracts data from three data bases: a scenario data base, a radionuclide inventory data base, and a data base of radionuclide properties.

The scenario data base contains release pathway descriptors for over fifty different release scenarios. These release scenarios were derived for the following phases of operation and post-operation: waste packaging, waste transportation, waste arrival phase (pre-entry inspection), on-site handling and trench emplacement, storage in an uncovered trench, waste burial (including backfill and compaction), post-burial (early time period, <100 years) and post-burial (later time period, >100 years). The 100-year breakpoint corresponds to an anticipated change in post-burial institutional controls.

The radionuclide inventory data base contains source terms for five sets of wastes: control rods and high activity components from light water reactors (LWRs); miscellaneous wastes (resins, sludges, trash, etc.) from LWRs; LWR decomissioning wastes; miscellaneous wastes from hospitals and similar institutions; and typical waste concentrations in a low-level waste shallow-land burial trench.

The radionuclide properties data file contains half lives, dose factors and gamma emission data (by gamma energy group) for over 350 radionuclides.

INPUT AND OUTPUT

Input data falls into the following categories: scenario and inventory selections, weather data, geologic data, demographic data and option switches. Of these, the geologic data tends to be the most bulky. We may, in the future, develop a geologic data file with element and soil type dependent coefficients from which BURYIT can extract the required soil data.

The output is the population or maximum individual dose given by organ, pathway, isotope, population age group, and radial distance from the source. Additional detail from the analysis process can be output on option.

CODE EXECUTION EXPERIENCE

BURYIT has been used to generate some sample cases and to perform some sensitivity studies, but has not yet been used to analyze any existing or proposed low-level waste disposal facilities. Execution times vary from a few CPU seconds on a DEC-10 computer for simple problems involving the calculation of only direct gamma exposure

to nearly an hour for complex problems involving many radionuclides, many soil layers and hundreds of repeated wet/dry cycles for chronic release problems involving groundwater transport and time periods of thousands of years. Typical problems require less than five minutes CPU.

In the sensitivity study, major variables affecting the result for a given airborne release scenario were the population, the agriculture and the weather pattern. Major water pathway sensitivity parameters were aquifer travel time and turnover and nuclide solubility.

Test cases for generic facilities indicated relatively high population doses from incinerator accidents involving the airborne release of respirable contamination. Chronic releases via soil water pathways tended to be small because of nuclide binding in the soil.

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MODELS AND CRITERIA FOR LLW DISPOSAL PERFORMANCE

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ABSTRACT

A primary objective of the Low Level Waste (LLW) Management Program is to assure that public health is protected. Predictive modeling, to some extent, will play a role in meeting this objective. This paper considers the requirements and limitations of predictive modeling in providing useful inputs to waste management decision making. In addition, criteria development needs and the relation between criteria and models are discussed.

PREFACE

This paper is a compilation and summary of informal remarks delivered to the LLW Modeling Workshop at Denver, CO in December, 1980.

INTRODUCTION

Calculational models for the prediction of the consequences of waste management activites should be consistent with applicable criteria; however, definitive criteria for judging the effectiveness of low-level waste management activities have not, as yet, been established. Despite the absence of official criteria, there has been a considerable amount of work on model development. Aside from the development of definitive criteria, there are several other areas that should be defined before beginning model development. Model development requires consideration of what is to be predicted, how accurate it must be, and how it can be validated.

Over three hundred existing models applicable to low-level radioactive waste have been identified.[1] Yet, an extensive degree of effort in model development continues. Given this situation, one might logically ask the questions: Why isn't what we have good enough?; What are the specific gaps that need to be filled?; and How can we recognize an acceptable model should one evolve? These questions should be resolved before more extensive model development takes place. Failure to do so could result in an endless quest for some unattainable state of perfection.

*This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

PATHWAYS FOR EXPOSURE

The determination of what processes are to be modeled requires the identification of pathways for human exposure to low-level waste materials. Figure 1 illustrates the major pathways of concern.

Water pathways are generally believed to be the most important pathways for human exposure. The two forms of water pathways are surface runoff and groundwater transport. Climatic conditions (arid versus humid) strongly influence the importance of these pathways.

The airborne pathways can result from operational release during waste disposal activities, release to the air through erosion, and release in conjuction with the evolution of gases in the waste material. The erosional release pathway is a consideration primarily during the post-closure phase of the disposal operation.

Intrusion is another potential pathway for exposure to LLW materials. Human intrustion can be either intentional or inadvertent. In addition, plant and animal intrusion present potential exposure pathways.

Other pathways include combinations of the previously discussed modes. For example, surface runoff followed by subsequent wind transport could be considered.

An important objective should be the identification of pathways so trivial that attention can be more reasonably directed to those which have a greater likelihood of transporting significant quantities of hazardous material to the biosphere.

MODELING APPROACHES

Considering the many potential pathways for human exposure, a review of previous modeling studies indicates that perhaps an inordinate amount of effort has been devoted to the groundwater pathways. This is particularly true in light of previous studies[2,3] which indicate that in terms of maximum individual exposures, the groundwater pathways constitute a relatively minor threat. Figure 2, taken from reference 2, shows the results of such a study.

There are several major approaches to the modeling of environmental transport. These include:

- Physical (Analytical)
- Empirical (Analog)
- Statistical (Probabilistic)
- Combinations

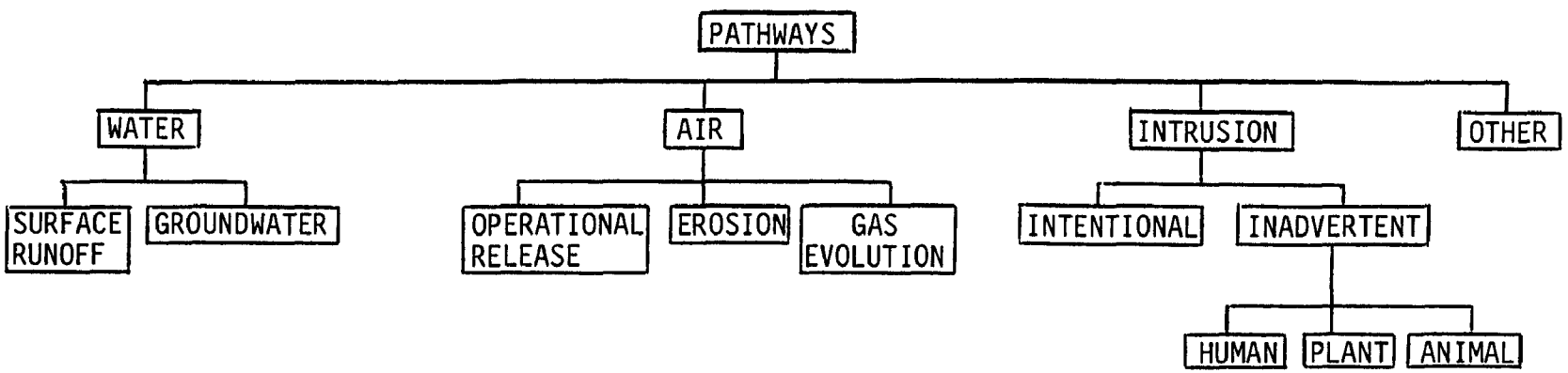
Physical models are determined by an analytical or theoretical description of the process being modeled based on first principles. Due to the infinite complexity of real world processes, physical models can never be exact predictive tools.

Empirical models are based on experimental data without the necessity for a detailed underlying theoretical basis. They represent an acceptance of the inability to thoroughly understand the process while making the best use of the data that we do have.

Statistical models use probabilistic inference to model the process. In some cases this is because the underlying theory is

Figure 1

Evnironmental Pathways for LLW



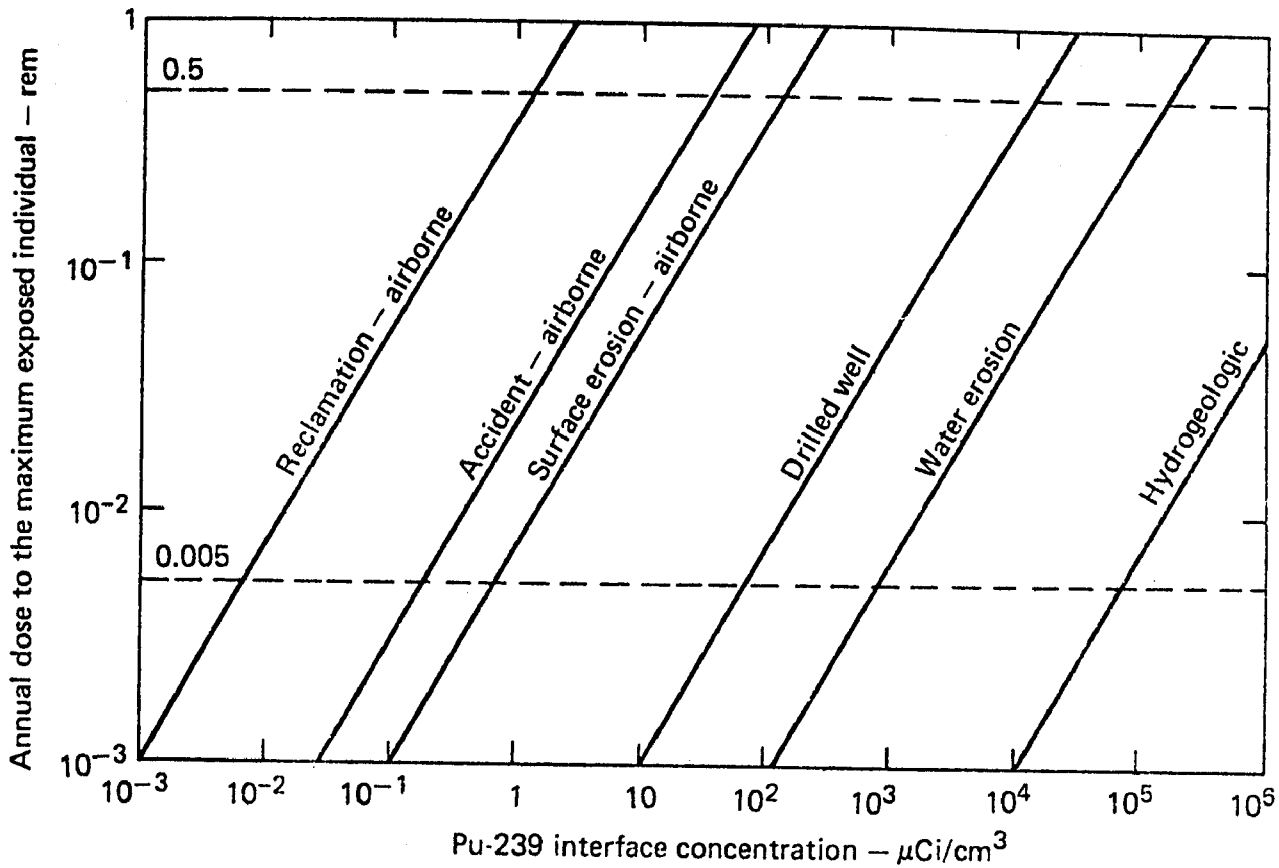


FIG. 2. Annual individual dose vs HLW/LLW interface concentrations for ^{239}Pu calculated for six exposure scenarios.

probabilistic in nature, and in other cases it is a reflection of the uncertainty about input parameters or the detailed underlying physics. Models may also use a combination of these approaches.

MODEL LIMITATIONS

There are several well known limitations to predictive modeling. These include data limitations (where the complexity of the model may outrun the available data), computational limitations (where the complexity of the model outruns the computational capabilities), and developmental limitations (where time, economic, or other factors limit the desirability or capability for model development). In addition, the apparent search for perfection in predictive modeling is not only unnecessary, but may even be counterproductive.

There appears to be a tendency in model development to equate the level of complexity and detail with the credibility of the results. Modelers should be cautioned to keep in mind the famous GIGO admonition (garbage in, garbage out). Model complexity should never be used to disguise either lack of understanding of phenomenology, or deficiency in quality of data input. No degree of model complexity or precision can compensate for a lack of either understanding or information in the analytical process.

VALIDATION

In light of these limitations, it is important to consider the question of model validiation. In the absence of experience (particularly the required observations over prolonged time periods) the process of validation is tenuous at best. How can we tell if a model works or not? One possible approach is to use natural analogs for the purpose.[4]

An application of this approach may be found in predictive modeling for the effects of Iodine-129 in radioactive waste. This radionuclide has been a source of concern because of its extremely long ($\sim 10^7$ yr) half-life.[5] A recent study[6] indicates that, as a result of groundwater leaching of high level waste, a maximum radiation dose of 3.3 rem/yr to the thyroid could result. Although we are unfamiliar with the details of the model producing this result, the prediction can be checked using the natural analog approach.

Assuming the high-level waste repository contained the waste from 10^3 GWe-yr of power production, it would have a total inventory of about 10^7 gm of I-129. Further, assuming the repository was 1000 m deep and sited in a watershed of 10^4 km^2, the total natural iodine inventory in the top 1000 m layer of earth would be about 8×10^{12} gm. If the iodine in the waste leaches at a rate no more or less than that in the soil, then, at equilibrium, the average ratio of I-129/total iodine is 1.3×10^{-6} at the point of groundwater discharge. Because of its low specific activity, it can be shown that if all the iodine in the human thyroid were I-129, the maximum dose to that organ would be ~19 rem/yr. Therefore an individual receiving his

total iodine intake from that watershed could receive a maximum thyroid dose of only $(1.3 \times 10^{-6}) \times 19 = 2.4 \times 10^{-5}$ rem/yr, or about five orders of magnitude less than the predicted 3.3 rem/yr. Although such predictive models are based on admittedly conservative assumptions, it might be in order to question the degree of conservatism. Excessive conservatism, sometimes bordering on the absurd, can call the entire modeling procedure into question.

CRITERIA

As indicated previously, the development of models in the absence of definitive criteria is problematic. Previously proposed guidelines have tended to be vague. Such guidelines are not very useful in planning the development of models.

While radiological protection should be the overriding concern, the approaches to the required analysis is sometimes confusing. Emphasis on the maximum individual dose results in "worst case analysis". Two deficiencies of the "worst case" approach are: (1) it is highly dependent on the imagination of the modeler in selecting his assumptions, and (2) to the non-professional, the result may appear to reflect reality instead of an extreme and unlikely situation. An approach toward eliminating this problem would be to incorporate the concept of probability into the modeling process. This approach requires the determination of probabilistic criteria.[7]

In any case, definitive standards are vital. If you don't know what you are looking for, the chances are that you won't find it. In addtion, predictive modeling capabilities should not dictate criteria - it should be the other way around.

SUMMARY COMMENTS

Definitive criteria are essential in the planning of waste management activities. In particular, the strategy for model development in support of the LLW program would logically depend on the prior establishment of criteria in order to ensure reasonableness and consistency.

Model development should take into account the question "how good is good enough?" in addition to pathways (what is to be modeled) and approach (how to do it). Recognizing the limitations of the modeling process, it should also be noted that models are tools to assist in the decision making process. They should not be considered to be an end in themselves.

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Workshop Summaries

SUMMARY OF RELEASE MECHANISMS WORKSHOP

L. R. Dole,[†] Chairman
D. E. Fields,[‡] Secretary

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Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

The purpose of this workshop was to identify the parameters that control the release rates of radionuclides from low-level waste (LLW) shallow land burial sites in which radioactive waste has been and will be placed. This panel (for participants, see Appendix A) searched for deterministic relationships describing source terms for the low-level waste trenches whose components are waste forms, containers, backfills, and other "engineered" bariers.

The need for this release mechanisms workshop was established in a previous group of workshops [1], during the special Interagency Meeting on Low-Level Waste Environmental Modeling in Bethesda, Maryland, July 30-31, 1980. All three July 1980 workshops, (1) Model Status and Development, (2) Validation and Verification, and (3) Criteria for Selecting and Applying, declared the inadequacy of the present description of the low-level waste disposal site source terms, and the lack of models describing the leach mechanisms and the chemical forms of potential contaminant releases, resulting from shallow land burial sites containing LLW.

Therefore, the goal of this panel was to discuss the past experience and ongoing research concerning the chemical, biological, and mechanical processes summarized in Table 1.

Due to the makeup of the panel, discussions focused most sharply on Mechanical Processes. Based on several field studies at existing burial sites and operating experiences, the discussions summarized below (1) described the three common site geologies, (2) identified subsidence-driven scenarios, (3) identified site surveillance requirements, (4) determined the present "state-of-the-art" of *in situ* source term characterization, and (5) outlined the course of action to effectively improve our quantitative understanding of release from LLW burial trenches.

The panel was skeptical that one "standard site model" could deal with the range of geological and climatological settings in which LLW

Table 1. Processes Related to Radionuclide Releases from Low-Level Shallow Land Burial Sites

1. Chemical Processes
a. Leaching of waste forms
b. Canister corrosion and degradation
c. Nuclide speciation, complexation, etc.
d. Nuclide retardation in backfill systems
e. Others
2. Biological Processes
a. Barrier degradation
b. Mobilization of fission products and actinides
c. Gas generation
d. Others
3. Mechanical Processes
a. Compaction and subsidence
b. Failure of barriers
c. Water penetration of capillary barriers
d. Others

burial sites are placed. A minimum of three typical settings were considered. First most sites west of longitude 100°W are located in porous host rocks and in semiarid to arid climates. Since these sites generally lose more moisture through transpiration than is received from precipitation, there is little or no hydraulic gradient under normal conditions.

Conversely, the two classes of eastern sites receive up to forty inches of annual precipitation. The permeable eastern sites are located in a range of hosts from sandy soil to fractured shales. On the other extreme, the third site classification includes eastern sites located in clay sequences in which essentially no permeability can be measured.

Burial site operators from all of the above classes of burial sites reported subsidence in their trenches. The impact of this subsidence on the trench cover has ranged from minor fissures to gaps that a man could fall into. In isolated cases, the trench contents were visible. These cases have ranged from potential to actual short circuits of the pathway to the biosphere.

The panel considered that the probabilities and consequences of subsidence features generally represented a more significant risk than ground water scenarios. Subsidence short-circuit scenarios include: (1) funneling run off through the trench, accelerating ground water contamination, (2) flooding and overflowing of the trenches, delivering activity to the ground surface, and (3) exposing the waste to weathering.

Operating practices have been developed to mitigate some of the causes of subsidence listed in Table 2. While vibratory compaction techniques have proven effective in filling voids and providing dense backfills, there are problem wastes and some subsidence is inevitable.

Table 2. Causes of Waste Burial Trench Subsidence

1. Compaction of the waste forms
2. Failure of backfill to fill voids between containers
3. Compaction of loose backfill material
4. Degradation of the waste by corrosion, biological decay, and dissolution

Therefore, a surveillance and trench cap repair program is required for at least the first ten years after the trenches are closed. It is conceivable that a trench subsidence surveillance program should be carried on for upwards of 50 years.

Panel discussion explored the possibility that trench cover fissuring may have more severe consequences in sites in impermeable formations. At first glance, the "mother nature" permeable systems, which rely on long travel times into and through the ground water to the biosphere, appeared less vulnerable to the short-circuit delivery to the ground surface from an overflowing trench — the so-called "bath tub effect." However, the permeable sites are still subject to flash flooding and are not exempt from this scenario. Also, disposal in an impermeable host is highly desirable since travel times can be measured in geological eras.

The potential "bath tub" scenario does not preclude sites in impermeable hosts. It does demand that the trench covers be designed carefully, that waste forms that do not contribute to subsidence are used, and that there is a rigorous surveillance program. Nevertheless, impermeable sites are good choices for the very long-lived nuclides.

In an attempt to cover the processes in Table 1, the panel explored the results of site studies, which included ground and trench water sampling and trench exhumation. In spite of the diversity in waste forms and sites, there were some consistent observations.

Shallow burial trenches generally are deep enough to insure anoxic reducing conditions. With the exceptions of rare geochemistries and aggressive reagents inside drums, corrosion of normal carbon steel can be slow. There are cases of intact drums older than 10 years. Even the biodegradation of clothing and cardboard at a South Carolina sites was small after 10 years.

The inhomogeneity of the waste is an insurmountable problem. Most of the trench contents are there because they were suspect and may have less activity than the dirt that was moved to bury them. It has been observed that 90% of the activity in a particular trench was in one small group of boxes, which represented a negligible contribution to the volume of the waste buried.

Regional ground water sampling, because of long travel times, is a very long-range effort. It is difficult to obtain representative trench water samples because of capillary holdup in the waste host, which results in poor flow distribution through coarse sump materials. While a "bath tub" trench might make leachate more readily accessible, the inhomogeneity of the trench contents makes an overall quantitative accounting questionable.

Nevertheless, attempts have been made to correlate the radionuclide inventories from hopeless shipping records and the activity in trench waters. Table 3 presents the guesstimates of yearly fractional release (FR).

Table 3. Estimates of Yearly Fractional Release (FR) from LLW Shallow Land Burial Trenches

Site	FR
Savannah River	10^{-8}
Oak Ridge	10^{-6}
West Valley	2.5×10^{-4}

The uncertainty range in the FR of four orders of magnitude cannot be reduced in the present situation. In the case of the existing trenches as they are found, both the inhomogeneity of the contents and the uncertain nuclide inventories preclude the possibility of refining our quantitative understanding of releases.

There are two solutions to this dilemma. The first requires two assumptions. These are (1) that the nuclide retention in the trenches is insignificant in respect to the travel times to the biosphere, and (2) that the chemical buffer capacity of the host is sufficient to overcome any adverse chemical effect on the nuclide retention from the trench contents. These assumptions reduce the LLW trench source term problem to estimating inventories.

The second course of action involves a ten-year research program. This program entails selecting sites and waste categories, segregating the waste, assaying the nuclide content, and preparing study trenches. Because the processes controlling the source terms are slow, the *in situ* study requires at least ten years. This field data will require an elaborate laboratory back-up study in order to interpret the results in terms of quantitative deterministic algorithms which are based on specific release mechanisms.

In summary, the decision to institute a lengthy, costly, and complex study balances against the potential impact of a regulatory decision requiring expensive waste conditioning and, possibly, extensive remedial treatment of buried waste.

In the previous workshops, the premise was stated that a model must first simulate before it can predict. This workshop indicated that a data base to successfully test a simulation does not exist in the case of shallow land burial. Furthermore, this workshop concluded that such a data base is not likely to be generated from current burial sites.

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APPENDIX A

List of Attendees
RELEASE MECHANISMS WORKSHOP

Name	Location
E. L. Albenesius	Savannah River Laboratory
Jim Bennett	U.S. Geological Survey
Clinton M. Case	Desert Research Institute
Don A. Clark	U.S. Environmental Protection Agency
Richard Codell	U.S. Nuclear Regulatory Commission
Leslie R. Dole	Oak Ridge National Laboratory
Ken Erickson	Sandia Laboratories
David E. Fields	Oak Ridge National Laboratory
Jesse Freeman	U.S. Nuclear Regulatory Commission, WM Uranium Recovery
Gerry Grisak	Environmental Canada, National Hydrology Research Institute
Cheng Y. Hung	U.S. Environmental Protection Agency
Donald Jacobs	Evaluation Research Corporation
Thomas Johnson	Illinois State Geological Survey
Craig A. Little	Oak Ridge National Laboratory
Steve Phillips	Rockwell Hanford, Research and Engineering
David E. Prudic	U.S. Geological Survey
Andrew E. Reisenauer	Pacific Northwest Laboratory
George Saulnier	TRW, Inc.
Jacob Sedlet	Argonne National Laboratory
Robert W. Thomas	Los Alamos Scientific Laboratory
Edwin P. Weeks	U.S. Geological Survey
Ken Whitaker	Chem Nuclear Systems, Inc.
Charles R. Wilson	Lawrence Berkeley Laboratory

SUMMARY OF WORKSHOP ON OVERALL SYSTEMS MODELING

James G. Steger, Workshop Chairman
Los Alamos National Laboratory
Los Alamos, NM 87545

Leroy E. Stratton, Workshop Secretary
Oak Ridge National Laboratory
Oak Ridge, TN 37830

This workshop was tasked to look into the need for and status of overall systems modeling for low-level waste. In attendance were 15 modelers, 6 managers/users, and 5 people who claimed to be neither of the above.

The approach consisted of providing the attendees with a written list of 10 questions that were to be discussed in sequence. A consensus position was to be obtained on all of the questions. The following is a brief summary of the results.

Q1. What needs to be modeled? What submodels are needed?

This question led to a discussion that lasted in excess of one hour. It was concluded that there need to be three different levels of models.

I. Screening Model. A need exists for a single overall screening model to make a first-order assessment. It should be able to be expanded and improved upon as experience is gained in its use. Probabilistic models should be considered as well as deterministic models.

II. Site Evaluation. A more detailed level of models to evaluate sites that pass the screening test is necessary. These models should have submodels for source term, airborne pathway, surface pathway, subsurface pathway, biological pathway, and human intrusion.

III. Process/Mechanisms. Researchers trying to understand the many processes/mechanisms involved in low-level waste disposal will have needs for many models in their work to test theories, explain experimental results and communicate with other researchers. These models will be quite specific to the problem being investigated.

When applying models as a predictive tool for evaluation, the three kinds of models listed above should be used in a hierarchal sequence. If the simple screening model with conservative parameters shows that there are no problems, then the modeling effort should stop. However, if there is an

indication that limits are being approached, then a more detailed analysis should be performed.

The group did not feel that the status of modeling was adequate and did not agree with the DOE comment (see Large, this volume) that no more models are needed. The group also cautioned that there seems to be an over-emphasis placed on groundwater pathway modeling.

Q2. Should the coupling of models proceed, and if so, how?

Coupling of models requires that they are capable of interacting. In the case of Screening Models, they can probably be coupled, but this level of detail is not necessary. Simple input/output relationships are adequate. For Site Evaluation Models, the pathway models are not sufficiently developed to permit complete coupling. For Process/Mechanism Models, coupling is problem dependent and desirable in some cases.

Q3. Are different systems models needed for arid vs. humid sites? For every site?

A single model can probably be developed for screening purposes for both arid and humid sites. However, there are enough differences between the arid and humid sites that a single site evaluation model does not seem likely. It is desirable though that effort should be made to keep the form and scope of these models as similar as possible to facilitate comparison of the results. For process/mechanism modeling, specific models will be required.

Q4. What determines when models for a specific pathway are adequate?

This question generated considerable discussion, with the final conclusion that the user must determine when a model was adequate. A model is a tool to help managers make decisions. The adequacy of the tool will usually be proportional to the amount of time that the modeler and user spend communicating. Once the user specifies what he needs and the modeler understands these needs, it is up to the modeler to assure model internal consistency and the proper balance between components.

Q5. What level of accuracy should we target for?

As in the previous question, this question can only be answered by the user. In any event, the status of modeling today will only permit making relative comparisons. Obtaining absolute values are beyond present capabilities.

Q6. Can enough data be obtained on an economical basis?

For Screening Models, enough data are already available or relatively easy to obtain. The answer is not so clear for the Site

Evaluation Model. Data will usually be obtainable on an economical basis, but in some cases the data will be very difficult to acquire. Process/Mechanism Models are usually designed to achieve complete understanding and consequently usually require more data than is easily obtainable. One caution was discussed at this time, and that is that care must be used in taking data from other sources to use in a model. Unless it is clearly understood how and why the data were obtained, it is very easy to misuse others' data.

Q7. What is the major purpose of an overall systems model(site evaluation, evaluation of operations, licensing, design of monitoring systems)?

This question is probably not appropriate for the group's consideration. Models contribute to all aspects of the problem, and it is not clear how one judges what the major purpose is to be.

Q8. Can post-operational performance be modeled and predicted using preoperational data?

The group felt that the answer to this question was yes with the present level of experience and data, but recommended that monitoring data be used to adjust the model as necessary to keep it as accurate as possible. Man-made modifications can be modeled better than making predictions of nature's actions in the long-term (300 years).

Q9. Do the models have the capability to handle different fuel cycles?

It was concluded that a different fuel cycle would not make the problem any more difficult and therefore the answer to this question is yes. The main problem at this time is obtaining adequate information on waste properties and release mechanisms.

Q10. Are there any models that propose to include such processes as transportation, regional siting, etc., for optimization of sites? Are such models desirable?

The group did not know of any total systems models (generation to dose-to-man), and felt that it would be unrealistic to try to include all of these factors in a single model. For additional information, several independent efforts are underway, which consider parts of the overall system. EG&G is developing a waste generator system model. Sandia is developing a transportation model. USNRC is preparing an environmental impact statement to assess the impact of the requirements of the proposed 10 CFR 61.

SUMMARY

The group was very enthusiastic about the exchange which took place. It is very rare when a working modeler can have a direct conversation with the policy setters in the DOE, NRC, EPA, and USGS, as well as his peers at the same time. There were many comments concerning how valuable the workshop participants felt that the exchange this meeting facilitated was.

There was surprisingly little difference of opinion or views remaining after discussion and resolution of terminology. Possibly a glossary of terms would be useful. Communication was a constant theme on almost every question. Everyone agreed that it needs to be improved. The data gatherers, model developers, and manager-users must fully understand each other's needs and capabilities.

The issues of model adequacy and accuracy cannot be determined by either the modelers or the users alone. There is a limit to what a modeler can do, and the user must identify the minimum needs. Close interaction is the only sure way to obtain satisfactory results.

The most serious limitation to overall system modeling is the lack of information about waste properties and release mechanisms. There are many different waste types and many different disposal environments. This situation makes for a very complex series of possible actions and reactions, which are impossible to model with existing data. Possibly the only solution is to pretreat the waste and to tighten the specification on disposal practices.

The final comment and the unanimous opinion of the group is that there is a critical need for standards to be used as targets. Until one knows what needs to be accomplished, it is difficult to determine how best to get there or whether or not success has been achieved.

APPENDIX A
Overall Systems Modeling Workshop Participants

Name	Affiliation
Richard Codell	U.S. Nuclear Regulatory Commission
Paul Dickman	EG&G Idaho
David Grove	U.S. Geological Survey
Ed Hawkins	U.S. Nuclear Regulatory Commission
Richard Healy	U.S. Geological Survey
Richard Heystee	Ontario Hydro
Preston Hunter	Ford, Bacon & Davis
Tim Jones	Battelle Pacific Northwest Laboratory
Dan Kapsch	Monsanto Research Corporation
Ken Kipp	U.S. Geological Survey
Eric Lappala	U.S. Geological Survey
D. H. McKenzie	Battelle Pacific Northwest Laboratory
Jim Mercer	GeoTrans, Inc.
Lew Meyer	U.S. Environmental Protection Agency, Office of Radiation Programs
Bruce Napier	Battelle Pacific Northwest Laboratory
Yasuo Onishi	Battelle Pacific Northwest Laboratory
Fred Paillet	U.S. Geological Survey
Dave Pollock	U.S. Geological Survey
Jack Robertson	U.S. Geological Survey
John C. Rodgers	Los Alamos National Laboratory
Bob Root	Savannah River Laboratory
Dale Smith	U.S. Nuclear Regulatory Commission
J. C. Sonnichsen	Westinghouse Hanford
Jim Steger	Los Alamos National Laboratory
Jim Stoddard	Science Applications, Inc.
Leroy Stratton	Oak Ridge National Laboratory
Burnell Vincent	U.S. Environmental Protection Agency, Solid Waste Office
G. T. Yeh	Oak Ridge National Laboratory

SUMMARY OF WORKSHOP ON ENVIRONMENTAL TRANSPORT PARAMETERS AND PROCESSES

E. L. Albenesius, Workshop Chairman
Savannah River Laboratory
Aiken, South Carolina 29801

C. A. Little, Workshop Secretary
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

ABSTRACT

This workshop was held on the afternoon of December 3, 1980 in Denver, Colorado. Nearly thirty participants discussed aspects of modeling the environmental transport of radionuclides from low-level radioactive waste shallow land burial grounds to the receiving human populations or individuals. Pathways of transport considered included groundwater, surface water, the atmosphere, and food chains. The ability to model transport in these pathways was discussed. Several modeling and data needs were brought to light and several recommendations were made to regulatory and funding agencies.

INTRODUCTION

The Workshop on Environmental Transport Parameters and Processes was held on the afternoon of December 3, 1980 at the Denver Marina Hotel, Denver, Colorado. Approximately thirty individuals participated in the discussion; their names and affiliations are listed in Table 1. The topics of discussion were limited to those that considered only transport from the trench boundary to some human receptor. Processes occuring within the trench were discussed in the Workshop on Release Mechanisms. Questions of accuracy and precision were largely discussed in the Workshop on Model Verification and Validation.

PURPOSE OF THE WORKSHOP

The ultimate purpose of this workshop, as well as the complete meeting, was to foster communication and cooperation between the various regulatory and funding agencies, model users, and model builders. In more specific terms, the purpose of the workshop was to

Table 1. List of Attendees of Environmental Transport Processes Workshop

NAME	AFFILATION
Ed L. Albenesius	Savannah River Laboratory
Clinton M. Case	Desert Research Institute
Don Clark	USEPA-Kerr Environmental Res. Lab.
Ken Erickson	Sandia National Laboratory
David E. Fields	Oak Ridge National Laboratory
Jesse Freeman	USNRC
Richard Heystee	Ontario Hydro
Cheng Y. Hung	USEPA
Craig A. Little	Oak Ridge National Laboratory
James Mercer	Geo Trans. Inc.
Bruce Napier	Battelle Pacific Northwest Lab.
Yasuo Onishi	Battelle Pacific Northwest Lab.
David Pollock	USGS
Andy Reisenauer	Battelle Pacific Northwest Lab.
Bob Root	Savannah River Laboratory
George Saulnier	TRW, Energy Systems
Jacob Sedlet	Argonne National Laboratory
James Stoddard	Science Applications, Inc.
R. G. Thomas	Los Alamos National Laboratory
Edwin P. Weeks	USGS
Charles Wilson	Lawrence Berkeley Laboratory
Ken Whitaker	Chem-Nuclear Systems, Inc.
G. T. Yeh	Oak Ridge National Laboratory

discuss the role in modeling of groundwater, surface water, and atmospheric transport processes and assess the relative importance of each of these processes, the adequacy of existing models and data bases, and the needs for further development. Table 2 lists the processes and pathways considered by the workshop participants. As mentioned earlier, processes occuring within the boundary of the trench were specifically excluded from discussion by this workshop, but were dealt with in the Release Mechanisms Workshop.

SURVEY OF MODELS

In an attempt to ascertain the state-of-the-art of environmental transport modeling for low-level waste management, a pre-workshop survey form was sent to each potential participant several weeks prior to the Denver meeting. The survey form is appended to this summary (Appendix A). For each pathway or process, respondents were asked to submit names and characteristics of environmental transport

Table 2. Pathways From Burial Ground Site to Man and Processes That Were Considered by the Workshop

Groundwater Transport

Surface Water Transport

Resuspension

Atmospheric Transport

Irrigation

Food Chain Transfer

Direct Exposure

models with which they were familiar or had experience. This exercise resulted in only a dozen model replies. Models were identified for only three categories: groundwater, atmospheric transport, and dose-to-man or "systems" models. These replies are tabulated in Appendix B, Tables B.1 - B.3. The groundwater model capabilities ranged from one-dimensional to multidimensional simulations of either water flow or transport of radionuclide decay chains. The atmospheric codes listed included both chronic release annual average models (AIRDOS EPA) and accidental release models (CRAC). The dose-to-man models all included some representation of the transport simulated by the groundwater and atmospheric models. None of the models in Table B.3 are presently documented in public literature. This is in contrast to the groundwater and atmospheric codes listed in Tables B.1 and B.2 which for the most part are documented in the available literature. This brief exercise suggests that, for low-level waste, dose-to-man modeling is much less well developed than either of the other types of modeling.

WORKSHOP DISCUSSION

Several questions were discussed during the course of the workshop. These included:

1. What is the relative ability to model each of the above pathways or processes?
2. What needs to be done to improve existing or future models of these processes?
3. If you were sponsoring the low-level waste modeling program for the entire nation, on what research would you spend your program budget?

These questions were posed to generate discussion among the attendees and for the most part were not answered directly or specifically. Nevertheless, answers were discerned for each model type during the ensuing discussion.

With regard to groundwater (GW) models, the point was made that GW flow and transport codes were often so detailed and numerically complicated that they have little utility for many regulatory uses. The SWIFT code, for example, may cost as much as $200 per run. Uses such as those by EPA where numerous sites must be screened would seem to preclude using a code that is expensive to run. It was agreed that, in terms of code development, the computer time was a small expense compared to either development manpower or data collection. The participants also agreed that, in general, the quality of groundwater models greatly exceeds that of the data used for input parameters (e.g., k_d, storage coefficients).

Surface water flow and transport models were also discussed. Onishi and his coworkers at PNL have recently reviewed 28 surface water models and their characteristics (Onishi et al., 1981) The group generally agreed that, with the exception of sediment transport, surface water models are collectively adequate or better. Sediment transport however, is not well developed. It was stated that models, especially assessment models, usually strive for description of average conditions and discount the effects of low probability events. For example, the James River model developed for the Kepone pollution case (Onishi and Wise 1978) has a deficiency in the inadequate treatment of pulsed input such as wash from severe flooding. In the case of a sediment transported pollutant, such as Kepone, the greater human hazard may be neglected if sediment transport resulting from low-probability events is not well modeled. The relatively long time frames of low-level waste modeling may make detailed modeling of either dissolved or sediment-attached pollutants unnecessary; dilution over total surface water flow may be acceptable with much less effort.

Consensus regarding atmospheric transport modeling was that the Gaussian Plume model (Gifford 1968) is the best known and most widely used model. The Gaussian Plume is reasonably accurate to distances out to perhaps 80 km from the source except for situations of complex meteorology. For modeling potential airborne impacts on humans from low-level waste burial sites, resuspension will be the most difficult process to model. Resuspension likely provides a large portion of the material input to the transported plume. However, resuspension models are at this point conceptually crude and for the most part only empirical models (see Healy, this volume). Data to parameterize resuspension models are also likely to be highly site-specific.

Food chain transfer models were seen to be a weak link in the modeling of transport from burial grounds to humans. This is the

case for two reasons. First, the models used to "transport" radionuclides through food chains are generally simplistic multiplicative chain or equilibrium models. For certain applications such as integrated doses to a static population over a long time period (several generations) these models may be adequate. However, for any application resulting from short term releases the models are crude. The second difficulty with food chain models is the lack of quality element-specific data for most of the transfer factors in the food chain (e.g., forage-to-milk transfer within cattle, gut-to-organ transfer within humans).

A consensus among the modelers was that credible scenarios of exposure need to be developed. So-called worst-case scenarios may need to be discarded for the simple reason that they are not always conservative; virtually any "worst-case" scenario may be made more damaging by employing less realistic assumptions. Scenarios for impact estimation from trench intrusion, site reclamation, on-site spillage, etc. are needed for modelers to construct reasonable modeling approaches. Many of the participants felt that some important regulatory decisions were being made by modelers by default when dose calculation scenarios were designed by modelers.

The environmental transport of radionuclides from a shallow land burial ground is very complex. Most of the workshop attendees agreed that the best use of modeling of low-level waste burial is as a screening device for the selection of potential new disposal sites. In this context, dose or risk estimates from models would be used in a relative sense and would not be considered estimates of the absolute radiological exposure or risk. Site selection and screening processes should utilize not only models but surveys of geology, hydrology, intuition, etc.

CONSENSUS OF THE WORKSHOP

The participants reached consensus on a number of questions and issues. Five statements of agreement are summarized in this section.

Modeling expertise is generally adequate for the perceived needs of modeling low-level waste environmental transport. However, some of the submodels need improvement. In particular, submodels of resuspension, sediment transport by surface water, and intra-trench processes that lead to radionuclides leaching out of the trench need conceptual improvement.

Even though modeling expertise is adequate, the predictive capability of the models perse is not satisfactory. The lack of faith in predictability arises from an awareness that the models do a poor job of estimating absolute values. The models are of great value in generating relative numbers. One such model application would be ranking the suitability of several alternative sites.

The participants agreed that to improve the ability to simulate a given site the greatest need is for a more complete data base. An example of needed types of data not readily accessible is given in Table 3. Operators interested in predicting the performance of a chosen new site would be advised to make an effort to acquire the listed data. Many of these parameters require site specific measurements and none of these data are readily available for presently unidentified sites. Some data, such as radionuclide inventory and physical form may be acquired through accurate record keeping. Others, such as dispersivity values are not even measurable quantities in the field, but are usually back-calculated from the results of a hydrologic flow model.

The workshop agrees that of the numerous models listed in several recent model compendia (e.g., Mosier et al., 1979), only a few codes, probably less than fifty, were adequately documented. Adequate documentation includes not only internal code comments, but also a comprehensive user's manual describing theory, operation, and a sample problem to check model results. It may also be a useful task for some group to specify the use of given models in given situations. In some ways this could be similar to the USNRC specifying its Regulatory Guide models. What group would be responsible for pursuing such an examination of models for low-level waste is unclear.

A final consensus of the workshop is that credible scenarios of human exposure to low-level waste buried in shallow trenches need to be developed. Definition of allowed human activities under such headings as intrusion, reclamation, etc. are, at present, not standardized. This lack of definition makes difficult the intercomparison of results from several models. Again, the location of the responsibility for developing scenarios is not clear.

Table 3. Necessary, But Not Readily Available, Data for Modeling Low-Level Waste Impacts at Hypothetical Burial Grounds

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Trench Contents
- Radionuclide inventory by activity
- Chemical form of elements
- Physical form of elements
- Presence of extraneous material (pesticides, herbicides, etc.)
- Distribution coefficients (k_d)
- Waste form interaction with biosphere

Geologic Characteristics
- Geochemistry
- Stratigraphy
- Fracture distribution

Hydrologic Characteristics
- Head distribution
- Sorption coefficients (in presence of expected groundwater chemistry)
- Conductivity (for both saturated and unsaturated conditions and in presence of expected groundwater chemistry).
- Porosity
- Dispersivity values
- Boundary conditions
- Water storage coefficients

Biological interactions (such as burrowing animals)

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Model Output

What is the model output? For a groundwater flow model it might well head distribution; for atmospheric transport, Chi/Q. Be as specific as possible.

Data

What input data are necessary for model/code operation? Are these data generic or site-specific? Are they presently available, included in the model/code documentation? Are the included data credible? Again, be as specific as possible.

Complexity

Is the model simple or complex? For example, solute transport models for groundwater may be 1-, 2-, or 3-dimensional and may include constant or changing chemical conditions. How about ease of operation?

Documentation

Is the model well documented? Are the assumptions clearly and completely stated? If the model has been coded for computer use, is the necessary machine-intrinsic information such as JCL explained? Is there an adequate user's manual? Is a sample problem included?

Reference

Give a complete reference to the model or code. If the work is ongoing, please list the site and principal investigator or contact persons.

Thank you for your cooperation.

APPENDIX A

PREWORKSHOP SURVEY FORM

Due to the shortness of time and the potentially large number of participants, it is imperative that this workshop be structured and focused. The ultimate goal of this and the other workshops is to foster cooperation and communication between the represented agencies and their contractors. A more specific goal is the determination of the state-of-the-art of and needs for environmental transport models useful for low-level waste management. As preparation for the workshop, would you please participate in the following exercise before arriving in Denver? The tables we produce will become an important source of information.

Please complete one of the following forms for as many applicable models as you wish (make additional copies if you need them). List those models which you have used or know of; they may be in development, well-known, for a single pathway, or "comprehensive."

You need not include every known model on your lists; we are interested in specific examples of the existing or developing environmental transport models so we can gauge where work is needed.

Please leave copies of your forms at the meeting registration desk in the hotel. The data you provide will be compiled before the workshop begins.

The following guidelines may be helpful:

Pathway or Process

Choose one of these (or add others): groundwater transport, surface water transport, resuspension, atmospheric transport, irrigation, food chain transport to humans, direct exposure, erosion, intrusion.

Model

Name a specific model or code of a model.

Model Type

Describe the type of model you have named. Possible entries might include Gaussian Plume model, linear compartment model, equilibrium model, time-dependent model, finite-element or finite difference solution technique. Many other entries are possible.

Pathway or Process:

Model:

Model Type:

Model Output:

Data:

Complexity:

Documentation:

Reference:

APPENDIX B

RESULTS OF PREWORKSHOP SURVEY

Table B. 1. Results of Pre-workshop Survey: Groundwater Models.

Name	Model Type	Output	Data Input	Complexity	Documentation
GETOUT	One-dimensional transport; axial dispersion	Ci/yr discharged in time and space	Sorption equilibrium constants; groundwater velocities; dispersion coefficient; height and width of input release band	Complex in dealing with numerical accuracy and decay chains; simple with regard to transport	Fair; well commented code; W. V. DeMier et al. (1979) PNL-2970
HYDRO	One-dimensional flow; finite element solution	Radionuclide concentration in soil in time and space; amount released to aquifer in time;	Site specific kd; sorption coefficients; multi-layer geological structure; water conductivities	Crank-Nicholson Finite Element solution; constant chemical conditions; constant solubilities	No formal document available; Bahram Amirijafari SAI
SWIFT	Multi-dimensional transport; finite difference solution.	Pressure, mass concent. or temperature in space and time;	Permeability, porosity etc., boundary and initial conditions	1-3 dimensions; radioactive decay chains; fairly difficult to use	Well documented; Dillon, Lantz & Pahwa (1978)
TRESCOTT	Groundwater flow; 3-dimensional finite difference solution	Hyraulic head and well draw down in time;	Initial head; storage coefficient; hydraulic conductivity; transmissivity; recharge; grid spacing.	Constant input; changing input parms for transient runs requires sequence of runs.	Well documented including theory, input description; Trescott, Pinder & Larson (1976)

Table B.2 Results of Pre-workshop Survey: Atmospheric Transport Models

Name	Model Type	Output	Data Input	Complexity	Documentation
AIRDOS - II AIRDOS - EPA	Gaussian Plume; analytical; chronic releases	Annual population and maximum individual dose	Extensive; includes population dist., annual average meteorology; agricul. data	Fairly simple to operate	Good; sample problem included; user's manual; Moore et al. (1979)
CRAC	Analytical; reactor accident releases	Population doses, latent and chronic; population fatalities and injuries; accident costs	Population and agricul. data; reactor releases inventory and release fraction; health effects parameters	Fairly large, but straight forward	Well-commented; documented in WASH-1400 Appendix VI. NRC (1975)
XOQDOQ	Gaussian Plume; analytical	X/Q or D/Q for either annual average or probabilistic	Site specific weather data, stack height (1977)	Fairly simple model	Rough draft document; Sagendorf and Gall

Table B.3. Results of Pre-workshop Survey: Dose-to-Man Models

Name	Model Type	Output	Data Input	Complexity	Documentation
BURYIT	Analytical; finite-element	Population doses	Site-specific geology, meteorology, pop. distribution	One-dimensional fairly simple	Early 1981; Science Applications, Inc.; David Lester
DITTYI	Multiplicative chain, equilibrium model	Integrated population dose	Scenarios; releases; population dist.	Many pathways; easy to use	Early 1981; Battelle-Pacific Northwest Lab.; Bruce Napier
DOSTOMAN	Finite difference and linear compartment	Compartment inventories vs time	Intercompartmental transfer coefficients	Easy to run	In-house documentation only; Savannah River Lab.; Bob Root
MAXI	Multiplicative chain; equilibrium model	Organ doses	Pathways; food consumption rates,etc.	Easy after first run	Preliminary user's mannual; Battelle Pacific Northwest Lab.; Bruce Napier
PRESTO	Analytical and multiplicative chain combination	Integrated pop. dose and individual dose; population health effects	Site specific geology, hydrology, meteorology, source inventory, pop. distribution; generic agricultural parameters	Easy to run; i.e. One scenario per run	1981; Oak Ridge National Laboratory; Craig Little

SUMMARY OF MODEL VERIFICATION/VALIDATION WORKSHOP

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INTRODUCTION

The goal of the Model Validation/Verification Workshop was to determine how the various agencies could best cooperate in establishing the credibility of models used in support of low-level waste management.

This workshop seemed particularly susceptible to problems of semantics. Definitions for such widely used terms such as verification, validation and calibration are not available. The group had the option of establishing a set of definitions or of finding a way of avoiding them altogether. The latter approach seemed to be the only practical option for such a short workshop. The discussion shifted from rigorous definitions to discussions of what each of us felt constituted "good modeling." The discussion focused on detailed accounts of actual modeling projects conducted by various participants. There was remarkable agreement among the group on methods and techniques used. It was soon realized that although each modeler may have a different name for each step in the modeling process, there was an underlying methodology common to all efforts discussed. The common concern of all modelers seemed to be to have their models and model results accepted. The basic ingredients needed to give a model credibility were identified as: (1) documentation, (2) reasonable estimation of important parameters, (3) mathematical checks, and (4) applications to independent data sets.

Participants (see Appendix A) felt that proper documentation of models was not currently available. Descriptions of models should include the usual information such as the equations solved together with the basic computer techniques used; however, more information is necessary. Explanations of the basic physical or empirical assumptions used to formulate the theory, examples of intended applications, and possibly subjective estimates of the overall value of the model are very valuable to model users. Documentation should include minimum computer requirements necessary to run the code, estimates of run time, and a detailed list of input data requirements. The discussion on making reasonable estimates of parameters brought up the subject of interaction with experimental and field personnel. The need for such interaction is so obvious it is difficult to discuss. There were no new ideas on how to foster more communication, but it was agreed that no modeling effort is complete without strong input from people with the proper physical insight and experimental data.

The last two items of the methodology list were handled together and resulted in the major recommendation of the workshop. It was recommended that the mathematical checks (number 3 above) and applications to independent data sets (number 4) should be accomplished by using standard test cases to cross-check most, if not all, waste management models. A good example cited for this type of activity was a recent Gordon conference sponsored by the petroleum industry where several models were applied to the same test cases so that model results could be compared. Members of the workshop who had attended this conference felt the technique was successful and could be applied to models used for low-level waste management. It was felt that test cases could be developed within major disciplines such as saturated and unsaturated flow, leach models, atmospheric transport, etc. A conference similar to the present interagency meeting could provide a forum for presenting the results of applying many models to the same test data. The expertise of most workshop participants was in the area of saturated moisture and solute transport. A detailed list of specifications that test cases should meet was developed and is presented below.

TEST CASES FOR MODEL INTERCOMPARISON

The description of a test case was divided into four areas: (1) data sources; (2) data specifications; (3) simulation specifications; and (4) points of comparison.

Data Sources

A primary source of data for making mathematical checks are the analytical solutions to the transport equations. While these data sets do not usually include complicated boundary conditions, they do provide valuable data on the ability of the computer code to solve the fundamental equations of interest. For more realistic data sets, it was felt that there was nothing wrong with hypothetical test data. If people experienced in the area of transport were given a chance, very realistic test cases could be produced which would closely resemble real world applications. This method seemed very useful for making relative comparisons between models while not being too useful for any absolute evaluation of a model's accuracy. The primary source of data for test cases is laboratory and field experiments. These data not only provide the most useful information for making absolute evaluations of models, but the constant use of field information in model development will also help prevent the development of models whose data requirements are unrealistic in terms of what is possible to do in the field.

Data Specifications

For the area of saturated moisture transport it was decided that the test cases should be three-dimensional (3-D) wherever possible. There

are sufficient 3-D models available to warrant this, and also 3-D data could be used in 1- and 2-D models by extracting the appropriate subset of data. The general consensus was that there is no need to worry about the non-isothermal cases for low-level waste. The test cases could be isothermal experiments. There were two fundamental data types which should be included. In hydrology models, it makes a difference if the data is cross sectional in nature or planometric. Different models are required for each type of data and test cases involving each type should be developed.

Simulation Specifications

In discussing test cases, it was most difficult for the participants to agree on the details of what scenarios and the specifics of what processes to include.

It was recommended that the specific radionuclides tritium, strontium-90, carbon-14, and uranium-238 should be included. It was felt that this list included sufficiently broad chemical and transport characteristics to be appropriate. An important feature of the simulation specifications is the form of output required. At a minimum, the output time should be fixed. If models are going to be compared to one another, they must produce equivalent output for the same time period. One cannot compare heads with flux or water level at two years with water level at two years and six months. The time scale of the test cases was discussed briefly and 300 years seemed reasonable. Obviously, no experimental data will be available for that time period, but test cases involving experimental data should be extended beyond the range of available data.

Points of Comparison

It is necessary to define exactly how the model outputs are going to be compared. This is not a trivial matter and can be the key to the success of the effort. One basic prediction of flow models is the direction of flow. Models that don't agree on anything else should still predict the same direction of flow. Mass balance is also a fundamental parameter of interest. While preserving mass balance is not a sufficient condition to accept a model result, it is necessary. If dispersion is being predicted, there are at least three measures to examine. The breakthrough time for the solute, the peak concentration over some time period, and an estimate of the overall fit to the concentration-time graph or concentration-space graph. A test procedure such as least-squares analysis may be appropriate. It should be clear from the outset what basis of comparisons will be. Other areas of comparison involve the computer characteristics such as language, CPU time, memory allocation, and the size of the time of a space step used in the simulation. There was some discussion about making a standard time and space step part of the simulation specification but no agreement was reached.

The important concept was that test cases could and should be developed to aid in the evaluation of models used in waste management, and it was recommended that there should be interagency cooperation in this effort. The discussion presented here is just an example of what the test cases for saturated water and solute flow might contain. A serious attempt at designing test cases would involve much more time and experts from many fields.

APPENDIX A

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MODELING AND LOW-LEVEL WASTE MANAGEMENT:
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*U.S. GOVERNMENT PRINTING OFFICE: 1981-740-062/102