017288
PC 7346809

MASTER

Contributions to
"DEEP GEOLOGICAL ISOLATION
OF NUCLEAR WASTE: NUMERICAL
MODELING OF REPOSITORY SCALE HYDROLOGY"

RECEIVED
APR 10 1980

for

University of California
Lawrence Livermore Laboratory

by

Michael D. Dettinger
Camp Dresser & McKee Inc.

April 1980

DISCLAIMER	
THIS DOCUMENT CONTAINS INFORMATION OF A PRELIMINARY NATURE. IT IS SUBJECT TO REVISION OR CANCELLATION WITHOUT NOTICE. IT IS NOT TO BE USED FOR ANY PURPOSE OTHER THAN THAT FOR WHICH IT WAS PREPARED.	
THIS DOCUMENT IS THE PROPERTY OF THE UNITED STATES GOVERNMENT. IT IS LOANED TO YOU BY THE UNITED STATES GOVERNMENT. IT IS NOT TO BE REPRODUCED OR TRANSMITTED IN ANY FORM OR BY ANY MEANS, ELECTRONIC OR MECHANICAL, INCLUDING PHOTOCOPYING, RECORDING, OR BY ANY INFORMATION STORAGE AND RETRIEVAL SYSTEM, WITHOUT PERMISSION IN WRITING FROM THE UNITED STATES GOVERNMENT.	

FOREWORD

The contents of this report are Camp Dresser & McKee's contribution to "Deep Geological Isolation of Nuclear Waste: Numerical Modeling of Repository Scale Hydrology," (FIN No. A-0277) submitted by Lawrence Livermore Laboratory (LLL) to the Nuclear Regulatory Commission as a report of the results obtained in the LLL Waste Management Program Task 3J, Post Sealing Phase Performance. Included herein are the contents of the third and fourth chapters and the technical appendix of that report which were produced by Camp Dresser & McKee staff members and provided to LLL for inclusion in their final report.

This report presents the results of CDM's technical consulting provided to LLL personnel performed under Purchase Order 7346809. It is the result of the extensive discussion and research carried out as a joint effort of CDM and LLL personnel to develop a modeling approach and to identify suitable models for application in the resolution of issues facing the NRC and in particular, for application in the analysis of the NRC's Priority 1 regulatory requirements.

Scope of Work

The Scope of Work undertaken by CDM covers three main tasks, described as follows:

- Task 1 CDM provided consulting services to the University on modeling aspects of the study having to do with transport processes involving the local groundwater system near the repository and the flow of fluids and vapors through the various porous media making up the repository system.
- Task 2 CDM reviewed literature related to repository design, concentrating on effects of the repository geometry, location and other design factors on the flow of fluids within the repository boundaries, drainage from the repository structure, and the eventual transport of radionuclides away from the repository site.

Task 3 CDM, in a joint effort with LLL personnel, identified generic boundary and initial conditions, identified processes to be modeled, and recommended a modeling approach with suggestions for appropriate simplifications and approximations to the problem and identifying important parameters necessary to model the processes.

Project Organization

CDM's services under Purchase Order 7346809 were provided under the direction and through the efforts of the project's Principal Investigator, Donald E. Evenson. The contents of this report were prepared by Michael D. Dettinger. Becky Wilson, Henry Evans, and Constance Morris provided technical and editorial support in the preparation of the report.

CDM personnel worked closely with Harry Lutz and Willard Murray of the Lawrence Livermore Laboratory in the development of the results presented herein and in the preparation of this report. Richard Martin of the Lawrence Livermore Laboratory provided valuable assistance in preparing the report.

Report Contents

This report consists of two chapters and an appendix. The first chapter (Chapter III of the LLL report) presents a detailed description and discussion of the modeling approach developed in this project, its merits and weaknesses, and a brief review of the difficulties anticipated in implementing the approach. The second chapter (Chapter IV of the LLL report) presents a summary of a survey of researchers in the field of repository performance analysis conducted by New Millenium Associates for the Lawrence Livermore Laboratory in November, 1979, and a discussion of that survey in light of the proposed modeling approach. The appendix is a review of the important physical processes involved in the potential hydrologic transport of radionuclides through, around and away from deep geological nuclear waste repositories.

TABLE OF CONTENTS

	<u>Page</u>
FOREWORD	i
I. DECOMPOSITION APPROACH TO REPOSITORY SCALE MODELING	1
The Hierarchy of Length Scales	1
Room Scale	5
Mine Scale	8
Intermediate Scale	10
Relationships Between Scales	13
Physical Processes Versus Length Scale	14
Model Simplification Through Choice of Model Scale	19
Coordination of Boundary Conditions	21
Development of a Consistent Analyses	27
Use of Iteration to Develop Consistent Analyses	28
Order of Analyses to Minimize Iterative Requirements	30
Development of Analysis Capabilities	32
II. SURVEY OF REPOSITORY SCALE CALCULATIONS OF NUCLEAR WASTE REPOSITORY HYDROLOGY	37
Discussions with the Research Community	37
Rockwell Hanford Operations	39
Battelle Pacific Northwest Laboratories	39
Electric Power Research Institute	40
Lawrence Berkeley Laboratory	41
Office of Nuclear Waste Isolation, Battelle - Columbus	42
Princeton University, Department of Civil Engineering	42
United States Geological Survey	43
Sandia Laboratories	44
Conclusions	45
Discussions of the Survey Results in Light of Proposed Decomposition Approach	46
III. PHYSICAL PROCESSES INVOLVED IN POST-SEALING REPOSITORY PERFORMANCE	49
Advective Transport	49
Diffusion and Dispersion	54
Fracture Flow and Advection Through Fractures	56
Dissolution and Precipitation	58
Sorption Processes	61
Thermal Effects and Processes	64
Radioactive Decay Processes	70
Conclusions	71
REFERENCES	73

I. DECOMPOSITION APPROACH TO REPOSITORY SCALE MODELING

Problems to be addressed in assessing post-sealing repository performance cover quite a range of physical scales. Some aspects of repository performance such as the effects of the details of room design and waste canister placement must be considered in terms of distances that are small relative to the overall repository dimensions. At the other end of the spectrum, the effects of room, corridor and shaft layout may be assessed initially on the basis of very coarse approximations and large distance scales. Typically, the physical processes which dominate various aspects of repository performance are dependent on the distance scales of interest. Although, as will be discussed in the next section, essentially the same processes are active over the whole range of distance scales. The relative importance of the processes, the parameter values describing the processes, and the nature of external factors regulating the processes vary considerably from scale to scale.

The Hierarchy of Length Scales

The repository as a whole is a very complex hydraulic, thermohydraulic, chemical, and thermomechanical system with many different processes active to varying degrees at different scales.

Rather than attempting to assess the entire repository performance problem at once or within the framework of a single view of the repository system we suggest that the repository be addressed in terms of three characteristic distance scales. The scales (Figure 1) are:

a. ROOM SCALE

3-D VIEW

b. MINE SCALE

3-D VIEW

c. INTERMEDIATE SCALE

PROFILE VIEW

Figure 1. Characteristic Distance Scales

1. Room scale, which includes only a rather small number of pillars and rooms within the repository structure,
2. Mine scale, which includes the entire engineered repository structure, and,
3. Intermediate scale, which includes that portion of the regional environs of the repository in which the repository may not be modeled as a point source to the surrounding regional flow.

It is expected that an understanding of repository performance at these three scales, along with an understanding of the interrelationships between the three scales, will be equivalent to a single, overall view of the repository system.

By working within this hierarchy of scales, the need for a single, overall model of the entire repository system is avoided. A single model conceptualization of the repository would have to include considerable detail at the room scale while extending over the entire volume described by the intermediate scale. On the other hand, the hierarchical approach narrows the point of view and addresses the salient characteristics of each aspect of repository performance. This approach results in much more manageable conceptualizations than the single model approach.

Immediately, a number of simplifications are available. Processes which are important at some scales but of only minor importance at the particular scale of interest may be neglected. The particular boundaries and geometries at the scale of interest may also suggest considerable simplifications. Thus, at the conceptual level, the simplifications introduced by a hierarchical approach are expected to be significant.

Decomposition of the repository performance problem according to the hierarchy of length scales listed above is also a reasonable response to the limitations of the practical tools with which repository performance analyses will be carried out. In practice, problems involved in assessing repository performance are of sufficient complexity that numerical models of repository systems will be the most accurate means of gaining understanding of the systems and factors affecting system performance. We expect that a numerical modeling approach based on the hierarchy of scales outlined above will be more productive and efficient than the single viewpoint alternative. As will be discussed in Chapter IV, some researchers in this field have concluded that the entire repository system can be numerically modeled quite effectively using methods that are available and being applied currently (Holland and Wilson, 1979); however, the cost would be enormous both in terms of computer time and storage requirements. As a result, current simulations of repository performance under generic conditions will be limited primarily by economic considerations. Simulations of specific repository designs at specific sites for screening or licensing purposes would also be limited by economics, but would be even more severely constrained by data limitations. Currently, the limitations are so severe that simple models of the repository system as a whole and/or fairly detailed models of limited aspects of the repository and its environs are the only tools that may reasonably be expected to be available for use in the short term. Very simple models allow economical simulations and have correspondingly simple data requirements. Unfortunately, the lack of detail in such models practically nullifies their usefulness. Detailed models of

limited areas or aspects of the repository system also allow economically feasible simulations and have less extensive (although more detailed) data requirements. If sufficient detail is included in such models and the relationship of the region of interest to the repository as a whole is properly accounted for, such models could be very informative. The decomposition approach to repository modeling makes use of detailed solutions of limited aspects of the repository and represents a workable approach within the limitations that currently constrain analyses of repository performance.

A crucial step in the decomposition approach to modeling and assessing repository performance is the development of links between the various scales. Without such links, a very incomplete model of the repository as a whole will result; with them, the resulting model will be equivalent to a single model of the repository at what is now an impractical level of detail. We expect that these links will be conceptual in nature and will not be included explicitly in the mathematical models themselves. The links or interrelationships will be discussed in some detail following a discussion of the three scales of interest.

Room Scale

An understanding of repository performance at the room scale allows many questions concerning the effects of small-scale construction decisions within the repository to be predicted. The room scale, as noted above, includes only a few rooms and pillars within the repository structure. At this scale, many questions regarding the civil design of the repository may be dealt with. The effects of room shape and size

are of interest at this scale. Questions of backfill and plug performance, as well as questions regarding the very local effects of heat loading patterns and waste canister placement may be addressed in large part at the room scale. These factors will tend to control the flow of groundwater, and therefore, the transport of radionuclides through the repository structure to potential pathways to surrounding aquifers and the biosphere. Design at this scale will also contribute to control of flow and transport within the repository medium, e.g., salt beds.

Finally, most of the actual observations of repository performance and properties will be conducted at this relatively manageable scale. Thus, room scale performance is a very important factor in the performance of the repository as a whole.

We suggest that, at least initially, the room scale be addressed in terms of either of two conceptual models.

One model of the repository at room scale might be a rather literal representation of the rooms and pillars of interest and the medium immediately surrounding them. This model would be based on some assumed permeabilities and other properties for the backfilled rooms and corridors and properties for the repository medium (e.g., salt beds). Given these properties and an appropriate set of boundary conditions, the conceptual model presents a somewhat complicated problem of mass transport through a porous medium in the presence of chemical, dissolution, and thermal effects. In order to model a region adequately, it is generally necessary to model a volume that is large enough such that processes of interest within the interior of the region are not dominated

by the particular type of condition specified on the boundary. Otherwise, only part of the effects of the processes of interest will be modeled and values specified at the model extremes will dominate results. The choice of boundary conditions for this conceptualization of the room scale will be difficult and will depend to a great extent on the results of analyses at the larger scales. The nature and importance of this dependence will be discussed in a later section.

The second conceptual model is based on the assumption that the repository medium (e.g., the salt bed) is essentially or totally impermeable. Under this assumption, the rooms could be modeled and the pillars and walls treated as boundaries of the problem. This assumption would drastically reduce the connection between the room scale problem and the larger scales, and therefore, the difficulty of obtaining boundary conditions. The assumption of an essentially impermeable confining medium would, however, be a reasonable approximation for only a few media. In salt, particularly domed salt, the assumption of impermeability might prove very reasonable. The permeability or impermeability of salt in situ has yet to be adequately explored, but appears to be extremely low. In most other media the assumption of medium impermeability ranges from being very poor to being a reasonable approximation, depending on the ratio of the medium permeability to repository backfill permeability. A ratio that is low ($\ll 1$) indicates a reasonable approximation, whereas a large ratio renders the assumption invalid. Notice that the above assumption of impermeability results in a boundary condition for flow and mass transport only. In the presence of thermal

effects, the assumption may lead to only minor simplifications unless further simplifying assumptions, such as isothermal flow, are made.

Mine Scale

The level of detail incorporated in analyses at the mine scale, which is defined to include the entire repository structure, should be adequate to allow assessment of the effects of repository configuration on post-sealing performance. At this scale the effects of the geometry and orientation of the tunnel system and the position and geometry of access shafts can be analyzed.

Repository failure modes resulting from large scale fracture formation, breccia pipe formation, shaft sealing failures, and undetected boreholes could be simulated at a reasonable level of detail. The potential for large-scale thermal convection and regional flow patterns to serve as driving forces for radionuclide transport through the repository structure and to the surrounding aquifers could be investigated best at this scale. The ability to simulate these factors in repository performance makes it possible to test the worth of many design features and specifications in confining radionuclides. At the same time, the ability to simulate the repository may well be the primary tool in deciding where and what to monitor in order to deduce the actual performance of repositories.

We envision models at the mine scale as sufficiently coarse that the rooms or even groups of rooms in the repository are treated as parallel-piped ("boxes") exhibiting essentially uniform properties. A room

averaged or "effective" heat loading parameter, permeability and transport properties, for example, would characterize each room in the structure. This simplification allows a large reduction in the amount of detail modeled. Currently, this reduction in detail is a practical necessity given the modeling capabilities available. The properties and processes retained under this simplification are those which control flow and radionuclide transport between the individual parts of the repository, both through corridors and through the confining medium. Processes governing flow and transport through the repository medium to surrounding aquifers may also be included. Thus, the simplified mine scale conceptualization models the interactions within the repository structure as a whole.

Mine scale models may range in level of detail from simple "box and shaft" models with the repository structure described by a single uniform parallelepiped with "effective" properties, to fully three-dimensional representations based on repository engineering design specifications. Between these two extremes, a variety of simplifications of the repository structure based on replacing groups of rooms with equivalent but simpler structures with locally averaged properties may be used.

As the detail incorporated in the mine scale model is increased, the specificity of the issues addressed by model analyses can be increased. The simplest of these models will yield only simple, approximate conclusions regarding the behavior of shafts and the effects of the general orientation of the repository structure. The "box and shaft" conceptual model, for instance, suggests, upon reflection, that in the presence of a

regional hydraulic gradient the potential for an access shaft to serve as a pathway to surrounding aquifers is reduced by situating it at the upstream margin of the repository. In the presence of significant thermal buoyancy effects, a number of more exotic shaft designs and repository orientations may be imagined on the basis of a "box and shaft" model to reduce the shaft's potential as a pathway.

Models in which large numbers of rooms are lumped into homogeneous, "equivalent" repository units (Holland and Wilson, 1978) may be used to address problems related to the general layout of the repository and the role that the major corridors of the repository structure play in radionuclide movement. Very detailed three-dimensional representations of the repository can be used to determine the role of individual rooms and corridors and other details of the layout plan on the overall performance of the repository.

Modeling mine scale processes to a level of detail that is appropriate in many cases may be expected to involve considerably more computational burden than most problems encountered at other scales. This is because the mine scale includes many more important details or components (e.g., hundreds of rooms at the mine scale as opposed to tens of geologic units at the next larger scale). Thus, mine scale analyses will generally face more pressing economic constraints than analyses at the other scales.

Intermediate Scale

The purpose of considering the intermediate scale is to bridge the gap between room/mine scale phenomena and large-scale regional phenomena.

The intermediate scale was defined above to be the distance scale which includes those parts of the regional groundwater flow system in which the repository cannot be treated as a point source of radionuclides. Generally, no matter what shape the repository is, at distances far enough from it, it is assumed that radionuclides will be transported as if from a source of radionuclides which is concentrated at a single point; that is, at such distances, it becomes impossible to deduce the details of the radionuclide source from the resulting concentrations. At smaller distances, radionuclide concentrations may be greatly affected by the areal configuration of the radionuclide release pathways. It is in this range that the intermediate scale lies. An understanding of repository performance at this scale will be important in deciding how repository siting and design can be chosen or regulated to minimize the capacity of regional groundwater flow to transport radionuclides to the biosphere or maximize radionuclide travel time in the event of a failure of the repository to contain the wastes.

The spatial extent of intermediate scale phenomena will depend on the repository design, the repository medium, and the discharge scenario. For instance, when the repository medium is a largely impermeable salt and the discharge scenario is shaft failure, the local scale nearly vanishes because the shaft's intersection with the surrounding aquifer serves as an effective point source of radionuclides. On the other hand, when the repository intersects or is intersected by a breccia blanket (Carpenter, et al, 1979), the release of radionuclides may take place

over a fairly extensive area. In the latter case, the effects of the release pattern may extend for distances of many repository lengths.

For the purposes of this scoping study, the intermediate scale situation is primarily of interest in those cases where the repository design affects the eventual regional transport of radionuclides away from the repository site. A scenario which fits this description very well is that in which the confining medium is relatively permeable, allowing transport from large areas of the repository through the repository medium into the surrounding aquifers. An example of this sort of scenario is the series of simulations reported in TM-36/21, "Groundwater Movement and Nuclide Transport" (Dames & Moore, 1978). In these simulations the expected temperature rise at the repository disrupts the regional flow for distances up to four repository lengths. Even if the confining medium is not permeable, thermal effects such as heat conduction away from the repository can disrupt regional flow and transport properties over long distances. Different heat loading patterns might be expected to diminish or increase this disruption and thus the design of the repository could be adjusted with this potential effect in mind.

Generally, an intermediate scale model is envisioned as representing the repository as a line segment, rectangle or rectangular volume embedded in the confining medium. Aquifers above and/or below the repository medium are modeled to distances at which the effect of the repository on pressure and/or temperature is small compared to repository scale effects. At these distances adequate boundary conditions can be estimated based on the ambient or regional trends in the system.

Relationships Between Scales

The modeling approach outlined above may be thought of as having two main elements:

1. development and/or application of models of the repository at the various scales, and
2. management of the relationships between the processes at the different scales.

In the above discussion, the individual scales were addressed. Inclusion of the relationships between scales in the analysis is crucial to the usefulness of model results. In the following paragraphs, the nature of the scale relationships, the reasons for their importance, and methods for dealing with them will be discussed.

Before proceeding with this discussion, it should be noted that the distinction between length scales will often be arbitrary. In the interests of clarity and order, a particular problem statement may be cast in terms of one distance scale or another, while in actuality, the situation lies somewhere between two distance scales. For instance, depending on the particular purpose of an analysis, the choice of whether a model represents the intermediate scale or mine scale may be indeterminate. In practice, this will not be a problem since a reasonably general model can be expected and designed to be effective when applied to any length scale. Thus, the suggestion of three distinct distance scales should not be understood to imply sharp boundaries between the scales. Rather, the scales are chosen solely for the purpose of dividing the many complex aspects of repository performance into a few broad, but not

mutually exclusive categories. These broad categories are individually much more manageable than the repository problem taken as a whole.

Physical Processes Versus Length Scale

In this section, the relationships between the decomposition approach and the physical processes which must be modeled to predict radionuclide transport within the repository environment will be discussed. Generally, it will be seen that most of the physical processes which are active in controlling or driving radionuclide transport at one scale are present at the other scales as well. The difference in the influence of these processes can most often be attributed to differences between parameters describing the processes and gradients driving the processes at the various scales. This section will deal with the physical processes in general. More detailed descriptions of the individual processes are presented in the Appendix. In particular, the nature of the relationships of process versus scale and their importance in the decomposition modeling approach will be discussed in this section.

A number of physical processes are involved in the potential transport of radionuclides through a repository and its surroundings during its post-sealing performance. In order to understand or predict overall repository performance, the effectiveness of specific design features and the effectiveness of monitoring strategies, these processes will have to be understood and the outcome of the more important processes predicted. The following geohydrologic processes will be active in determining repository performance:

- ° advective transport

- ° diffusion and dispersion
- ° fracture flow/advection
- ° dissolution and precipitation
- ° sorption processes
- ° thermal effects and processes.

The importance of these processes will vary from scale to scale and scenario to scenario. The role of each of the processes at the various distance scales is discussed briefly in the following paragraphs.

Advective transport, which is solute transport by the bulk motion of water, will be important in most media at all distance scales. This process will be much more dependent on the flow scenario than on the scale, but is generally the most effective, rapid means by which radionuclides are transported through the repository and surrounding geologic media. The other physical processes to be discussed will result in modifications to the flow field and rates of advection or will result in secondary modifications to the radionuclide concentration profiles as advection proceeds. Thus, the basic component of repository radionuclide transport analysis at all scales will be an advection model.

Dispersion, the mixing brought about by heterogeneities in the porous medium through which flow is taking place, plays a role in the transport of radionuclides which depends to a great extent on the distance scale of interest. Generally, a simple rule is that the dispersivity, a measure of the potential for dispersion, is roughly equal to the largest characteristic length of the heterogeneities. At the room scale, for instance,

it is expected that dispersion will be of somewhat limited importance with permeability heterogeneities on the order of centimeters long. These heterogeneities will include small-scale permeability variations in the repository backfill material and other small-scale permeability variations in those parts of the geologic medium on the boundaries of the repository rooms and corridors. At the mine scale, the effects of dispersion will be more extensive as substantially larger heterogeneities are included in the dispersion process. At this scale, larger scale variations (up to several meters in length) in permeability within the room and corridor network will be included in the dispersion coefficient as a result of the application of room-averaged "effective" flow properties. At the room scale, these details would probably be included in computations of advection rates and thus would not add to dispersion. Over the long distances involved in an intermediate scale model, considerable aquifer property variability is likely. This suggests that macrodispersive phenomena will be an important process. Aquifer variability at this scale will be on the order of tens of meters, and very large dispersion coefficients will arise. Some doubts have been raised about the applicability of the advection-dispersion equation in describing transport in this range. In most scenarios, however, it is expected that the errors incurred through use of this equation will not be so large as to nullify the benefits of modeling.

Prediction of the effects of flow through fractures in the repository medium presents a very complex mathematical problem which is handled differently according to scale and scenario. As noted above, advection

is a very important process in radionuclide transport; this is particularly true in the presence of fractures. Fracture flow/advection is extremely rapid regardless of scale and tends to dwarf other modes of transport. Although the potential importance of fracture flow is not so much a function of scale as of scenario, the choice between mathematical descriptions of flow through fractures will be based on the scale of interest and the amount of information available about the fractures at that scale. At the room scale, it will often be assumed that statistically few fractures are included within the model boundaries. Since a very large number of fractures must be averaged before the simplest representations may be employed (Freeze and Cherry, 1979), for small-scale analyses a complex statistical model will be required. At the repository scale, there is no reason to believe that the location and orientation of most of the fractures will be known. At this scale, if fracture flow is to be accounted for, other probabilistic fracture models or a Darcian model will have to be applied. An exception to this "rule" is the scenario in which one or a few large-scale (mine scale) fractures intercept the repository. In that case, the effects of the individual fractures must be accounted for. At the intermediate scale, a Darcian representation will often be a reasonable approximation for media in which fracture flow must be taken into account unless, again, a few important fractures must be analyzed.

The importance of dissolution and precipitation will be primarily dependent on scenario and will be important only in salt media. When large-scale dissolution is occurring, such as under conditions which lead to breccia

pipe or blanket formation (Carpenter, et al, 1979), these processes will be important at all scales. Under less catastrophic conditions, the processes will be important only at the room scale, if at all.

Outside of salt media, sorption processes are expected to be effective at all scales. Little change in the mathematical description or absolute importance of the processes should be expected from scale to scale unless the usual assumption of chemical equilibrium is violated. Non-equilibrium chemistry will dominate where travel times are very small; that is, in some room scale situations and in the presence of fracture flow. Under these circumstances the mathematical description of the effects of sorption on transport can become quite complex.

Under the term "thermal processes," we have included a wide variety of effects such as free convection, thermomechanical effects, and thermomigration. It is often very difficult to determine which of these processes will be important at a particular scale in a particular scenario. The thermomigration process may only be expected to transport radionuclides over very short distances (Evenson, et al, 1979) and we may conclude that this process will be important primarily at the room scale. It is generally difficult to predict the extent of convection and thermomechanical effects, although we suspect that individual thermal effects may be very important at all length scales. Generally, the parameters that control thermal processes are not functions of scale.

Finally, the importance of radioactive decay will generally increase with increasing distance scale, primarily because the characteristic travel

times tend to be longer at the large distance scales. Over the relatively short time periods involved in room scale analyses, decay will not have as significant an effect as it will have at the intermediate or regional scales.

To summarize, most of the physical processes controlling radionuclide transport through the repository system are present at all scales of interest. Several of the most important physical processes which may affect repository performance, such as advection and equilibrium chemical reactions within the porous media of the repository, are active in essentially the same way no matter what the scale of interest. These important processes are described mathematically in terms of the same governing equations and are of comparable importance at each scale. Other physical processes such as dissolution of the repository medium, fluid density and thermal buoyancy effects, although describable in terms of similar governing equations from scale to scale, may vary considerably in importance. Dissolution, for example, might be very important at the room scale and less so at the mine scale depending on scenario. Finally, a few processes, such as hydrodynamic dispersion, may not even be described by the same governing equations at all scales (Evenson and Dettinger, 1980).

Model Simplification Through Choice of Model Scale

Given the difference in importance of the various physical processes at different scales, it will often be possible to simplify repository analyses by concentrating on analysis at a length scale for which only the processes of interest are important. Under these conditions, the

other significantly less important processes may be neglected in analyses. For instance, a single model of the entire repository would have to include, in the general case, a mathematical statement of all processes as they occur at each of the scales, plus descriptions of their variations between scales. The complexity of such a modeling requirement suggests, once again, that the decomposition approach has very real advantages in the short term. Until we understand repository systems more fully, a real advantage of this approach is the potential it provides for limiting analysis to key issues and physical processes while maintaining a consistent view of the repository as a whole.

Although it will often be advantageous to neglect certain processes at a particular scale in repository performance analysis, it should be noted that most numerical model codes available are applicable to a wider range of conditions than is included in any one of the three scales outlined above. Because most processes may be described in terms of the same mathematical equations, regardless of scale, models tend to have a wide applicability. If no important processes at the scale of interest are neglected in the code and if nonlinear coupling effects between processes are properly accounted for, then the proper choice of model parameters, problem geometries, and boundary conditions become the critical points in application of the code. In fact, we propose to concentrate in the very short term on a single numerical model code for analyses at all three scales.

The SWIFT code, for example, deals with what we feel are the most pertinent processes (advection, dispersion, and hydrothermal effects) at

all three length scales. The governing equations will not change significantly over the range of distance scales discussed here and the code is expected to handle nonlinearities fairly well. Thus, this single model can be applied with only minor modifications for basic analyses at all three scales.

Coordination of Boundary Conditions in the Decomposition Approach

The proper choice of boundary conditions is essential to the development of consistent, meaningful analyses of repository performance using the decomposition modeling approach. Since the length scales into which we have divided the repository system are rather arbitrary, there is no reason to believe that processes in any one of the scales will be completely unaffected by the physical processes that are active at the others. In order to obtain a consistent view of the repository using the three distinct distance scales, it is necessary to include in the analysis at each scale some information concerning the results of processes at the others. Boundary conditions are the means by which this connection between scales is maintained.

Boundary conditions play a very important role in determining repository model results. For most processes included in a repository model, separate sets of boundary conditions have to be specified. The location, type, and parameter values describing boundary conditions must be chosen quite carefully to insure meaningful results.

Model boundaries must be located at distances far enough from the region of interest so that the properties are known or predictable regardless of

the results of the analysis. This is because predictions of an aspect of repository performance of interest will almost invariably depend on the boundary values applied. Obtaining an accurate solution under these circumstances is difficult, if not impossible. The proper location of boundary conditions to avoid this problem is generally discovered by iteratively solving the mathematical model with the boundaries of analysis located at different distances. The minimum distance beyond which model results are insensitive to further expansions of the boundaries is the most efficient location for applying the boundary conditions. As understanding of the system is improved, this iterative process for choosing boundary condition locations can be discarded in favor of educated decisions based on prior analyses.

There are generally a number of distinct types of boundary conditions possible for each process. For example, possible boundary conditions for flow through porous media may be the following types: specified head (or pressure), specified flow, or some hybrid combination of the two. The choice of boundary condition type should be based on whatever physical understanding of the system is available. First, a decision must be made regarding which properties are least affected by processes in the center of the model region; that is, in our example, is the flow field less affected than the pressure field at the boundaries or vice versa? Second, the boundary conditions which can be most accurately predicted should be preferred. Thus, if either specified head or flow boundaries could be specified for a particular analysis (depending on the choice of location) then the boundary condition type whose parameter values can be

most accurately specified should be applied. Boundary condition parameters range from numbers which directly specify the boundary value to parameters which indirectly specify the properties at the boundary. A specified flow rate is an example of the former, while a boundary permeability specified for certain leakage boundaries is an example of the latter.

As discussed above, boundary conditions must be located far enough from the region of interest so that the properties are not affected by the processes acting in the region of immediate interest. For this reason, fluid pressures, temperatures, and other properties at the furthest boundaries of a model of one scale are determined not so much by the processes acting at that scale, as by the processes at the next larger scale. For instance, the boundaries of a room scale model will be located at distances from the design feature being analyzed such that the various properties (pressure, temperature, etc.) are nearly unaffected by the design feature. That distance might include a few more rooms and corridors, or it might extend the analysis to a large part of the mine.

Rather than extending the analysis to this more complicated problem, that is, modeling large regions with room scale detail, one practical approach is to use information gathered at the next larger scale in the proposed hierarchy. Results of a detailed but more spatially extensive mine scale model can be interpolated to provide information for use in specifying boundary conditions for the room scale model. Underlying this interpolation is an implicit assumption that the properties properly chosen for room scale model boundary conditions are dominated by mine scale processes.

Thus, if the effects of a room size phenomena are to be entirely enclosed within the boundaries of a model, the boundaries will have to be far enough away that the rooms themselves will act as homogeneous "boxes" and properties that are "nearly unaffected by the room size design feature" are assumed to be roughly those found in mine scale considerations. The suggestion is not that the boundaries be moved outward until the entire area covered in a repository model is included; rather the boundaries may be chosen to include whatever part of the repository is affected by the processes of interest. Then the boundary values may be chosen with reasonable assurance on the basis of mine scale models in which the region covered by the entire room scale model represents a significant detail.

Generally, these external boundary conditions represent the link between analysis at one scale and the effects of larger scale processes. The preceding paragraphs have concentrated on the relationship between the mine scale processes and room scale boundary conditions. An analysis of intermediate or regional scale processes and mine scale boundary conditions would yield similar conclusions; that is, the boundary condition values specified for repository scale analyses should be the result of intermediate scale processes. Finally, the connections between intermediate and regional scale analyses are fairly clear and intermediate scale model boundary conditions should prove very simple to specify in terms of regional hydrologic conditions.

Other types of boundary conditions are internal "boundary" conditions or source/sink terms. These internal conditions are the values applied at

locations of the sources of the driving forces within the region of interest for the physical processes. If, as an example, thermal effects due to heat generated by the radioactive waste forms are the processes being analyzed, then a temperature or heat flow for each room or collection of rooms might have to be specified in order to proceed with mine scale analyses. These specified values would control to a very large extent the development and maintenance of convection currents, thermomigration, and the other thermal effects. At points in the region of interest other than the specified source or sink locations, temperature and other properties will be affected by both the source/sink conditions and the external boundary conditions and are part of what is solved for in the analysis.

Notice that in order to specify these source/sink boundary values, the effects of processes acting at smaller length scales must be at least partially understood. The amount of information about small-scale processes necessary to specify these averaged or representative values of driving properties will depend on the level of detail incorporated in the larger scale conceptualization; that is, a relatively coarse repository scale model would be insensitive to, and in fact unable to incorporate detailed information concerning the effects of room scale processes. On the other hand, the effectiveness and accuracy of very detailed models would be greatly enhanced by such information. Thus, depending on the level of detail incorporated in a repository scale thermal analysis, the specified values might range in form from simple average areal heat

loadings for the entire repository to specifications of the individual temperatures of each room.

In any case, it is clear that these source/sink values are intimately related to the smaller scale phenomena.

The "best" form and value that the source/sink conditions can take for any given analysis are those forms and values which will best include the effects of processes at the smaller scales on processes and results at the scale of interest. The nature of this "best" source/sink specification is very much a function of the scenario and aspect of repository performance being analyzed, and therefore, must be decided anew in each distinct case. In the case of a repository scale thermal analysis, the choice of a single room temperature value involves neglecting the actual variations of temperature within the room. Since thermal gradients and not absolute temperatures are often the important properties in thermal analyses, it is very easy to imagine a case where the most appropriate, or at least conservative choice of a room temperature would not equal the average temperature. A temperature biased toward either the maximum or minimum temperature expected in the room might be more defensible. Of course, where possible, a specified thermal gradient or heat flow would be the preferred internal boundary condition under these circumstances. Thus, a certain amount of experimentation with the forms and values of the source/sink terms in repository models should be carried out in order to insure that meaningful and defensible values are employed. As understanding of the system develops, the need for such experimentation will decline. It should also be noted that the choice of "equivalent" room

properties other than source/sink values, such as corridor resistances in flow models, will also require experimentation and justification since simple average values may not be truly representative of the effects of these properties when viewed from the larger scales.

In addition to their important role in models and analyses of repository performance at the individual length scales, boundary conditions represent the sole connection between phenomena at the various scales.

External boundary conditions represent the link between analysis at one scale and the effects of processes at larger scales while the internal source/sink boundary conditions represent the connection between this scale and processes at smaller scales. By means of these relationships, the performance of the repository may be analyzed and the role of individual segments of the repository analyzed in a physically reasonable context. In the next section, the means by which boundary conditions are used to insure meaningful analyses within the decomposition modeling approach will be discussed.

Development of Consistent Analyses Within the Decomposition Approach

The key to development of a meaningful, consistent model of the repository system as a whole within a decomposition framework is the realization that processes at each scale tend to exert a powerful influence in determining the boundary conditions of the next smaller and larger scales. Thus, within the hierarchical approach to decomposing repository performance analysis into more manageable problems, boundary conditions are expressions of their interrelationships between processes and phenomena at each of the scales. In this sense, the boundary values and

configurations are "coordinating variables" between the various levels of the decomposition of the system. The boundary values must be coordinated from scale to scale for a consistent picture of the entire repository problem to be developed; that is, all sets of boundary values must be consistent with the results of the other scales. Otherwise, a disconnected, potentially misleading view of the repository is developed.

If internal and external boundary values can be specified, analysis may proceed in isolation from the other scales; decisions regarding which processes to model and which methods of analysis to employ may be made. Generally, however, the boundary values are not trivially obtained, and may require a considerable increase in computational effort for the entire analysis. The proposed methods for arriving at consistent sets of boundary conditions and thereby arriving at consistent overall analyses of the repository will be discussed in this section.

Use of Iteration to Develop Consistent Analyses

External boundary conditions and source/sink terms at each scale are dependent to a certain extent upon the processes at other scales. This suggests that a certain amount of experimentation and iteration between scales will be necessary in order to develop a consistent analysis of the entire repository system within the framework of the hierarchy of length scales outlined above. In problems where all boundary conditions are heavily dependent on all other scales, a demanding iterative analysis will be required; that is, in some repository performance situations, in order to arrive at boundary values that agree from scale to scale, multiple analyses at the individual scales will have to be carried out.

In these iterative analyses, boundary conditions will be the "variables" iterated on with a converging group of increasingly consistent sets of boundary conditions being applied in each analysis. The iteration will consist of a series of primary and secondary analyses designed to experimentally determine and verify the proper boundaries and boundary values. The primary analyses are the analyses of the aspect of repository performance that is of interest to the analyst at the length scale of interest. Results of primary analyses based on a complete view of the repository system are the ultimate aim of this modeling approach. The secondary analyses are analyses which do not directly deal with the repository performance characteristics of interest at the scale of interest. Rather, these analyses are carried out solely for the purpose of developing information on which the boundary conditions for the primary analysis are based and by which these boundary conditions can be verified. For example, large scale analyses may play the role of secondary analyses for certain small scale primary studies by providing defensible external boundary conditions for use in the smaller scale analysis.

The "proper" boundary condition for a particular scenario may be obtained as follows: Using information about a boundary that is relatively well understood (e.g., regional conditions), secondary analyses are developed and carried out in an effort to develop projected conditions on which the primary analysis boundary conditions may be based. Since it is highly unlikely that both internal and external boundaries will be known at any one scale, the secondary analyses will be based on some guesswork. Thus,

if intermediate scale effects are being projected in order to obtain the external boundary values for a mine scale analysis, the expected regional conditions may be used to specify intermediate scale external boundaries, but the internal source/sink terms will have to be based on rough estimates of effects that will occur at the mine scale. Therefore, once the primary analysis has been carried out, the results will have to be checked to see that the internal boundaries employed in the secondary analyses are actually consistent with the small scale effects. If the initially assumed boundary conditions and those indicated by the results of the primary analyses are not in agreement, then the new boundary conditions or some compromise may be employed in a new round of secondary and primary analyses. This iteration between analyses at the various scales should continue until a consistent picture is achieved.

The amount of iteration between scales that is necessary will play a large part in deciding the efficiency of the decomposition approach to modeling repository performance. If analysis at each scale is very dependent on boundary conditions that are based on results of analyses at the other scales, then numerous iterations will be required to obtain results that are consistent at all scales. If too many iterations are necessary, then the immediate advantages gained by decomposing the repository performance problem into manageable scales of interest may be lost.

Order of Analyses to Minimize Iterative Requirements

Fortunately, we expect that for many analyses the interrelationships between several combinations of scales will not be strong or unmanageable.

For instance, intermediate scale problems have already been studied with reasonable results in the absence of a clear understanding of the smaller scale processes. Similarly, mine scale calculations are probably not very dependent, in many situations and scenarios, on detailed room scale results; many times the simplest of room-averages will be adequate.

Very often, the effect of choosing a particular source term will be much less critical, and the range of values that may reasonably be specified much more limited, than when specifying external boundary conditions. Even if detailed source boundaries are specified, their cumulative effects may be equivalent to simple averages and the importance of their variability very localized. In such cases, the details of the source terms may be of secondary importance and simple equivalent properties adequate. External boundary conditions, on the other hand, tend to have a more pervasive influence on analysis, providing the ambient conditions on which all smaller scale effects are superimposed. Because their effects are more pervasive, the details (or variability) of external boundary conditions are generally important, and a good understanding of the processes dominating them is necessary.

Because it is expected that the effects of external boundary conditions will be more pervasive and more effective in determining overall repository performance than internal source/sink boundaries, the number of iterations required to achieve consistency will generally be decreased if analysis is ordered so that large-scale analysis precedes small-scale analyses. Specification of the variability of external boundaries is

important and requires a reasonable level of understanding of the processes controlling them. Much simpler equivalent properties may be used for the internal boundaries. Thus, detailed understanding of large-scale processes must be developed before meaningful small-scale analyses can be carried out in any but a random trial and error fashion.

The most reasonable approach, therefore, seems to be to analyze the larger scale problem first, coordinating the small-scale problem to the larger through simple pre-analysis estimates of the small-scale properties. Once the large-scale analysis is complete, reliable external boundaries for the smaller scale problem of interest may be specified and the small-scale analysis carried out. Then, unless the small scale results are radically different from the pre-analysis estimates, the entire analysis may be considered complete. Since the large-scale problem "sees" the small-scale results as an internal source boundary with some average value, the large-scale analysis should not be very sensitive to minor differences between the pre-analysis room value estimates and the small-scale final analysis results. As a result, this strategy for coordinating the relationships reaches a consistent picture very quickly. In fact, for most analyses it is likely that single series of analyses from the large- to small-scale will be sufficient to obtain a degree of consistency that is adequate for the purposes of understanding the situation.

Development of Analysis Capabilities

Although a complete understanding of repository performance may require a thorough understanding of processes at all of the scales, many problems

can be addressed in relative isolation from one or more of the scales in the hierarchy. This will, of course, greatly expedite analyses. A number of important, albeit general, questions about the performance of generic repository design features may be analyzed immediately. Some generic questions of repository performance will be manageable without a complete view of the repository so that assurances that boundary conditions are consistent with larger scale views of the repository may not be necessary. In such cases, reasonable boundaries may be specified without recourse to extensive demonstrations of their validity. In other cases, the means by which the particular boundary values are maintained is less important than the reaction of the processes within the region of interest to them. The more complex questions that require an understanding of the interactions of the repository as a whole will have to be postponed until a greater body of knowledge concerning repository performance at all scales is gained. Generally, as analyses proceed, understanding of the repository system and methods of analysis may be expected to grow and the sort of questions addressed will increase in complexity.

There are a number of situations in which relatively isolated analyses at individual scales may be useful. As mentioned above, the larger scale repository analyses will often be relatively insensitive to small-scale effects, processes, and parameters and thus can, and in fact, have been analyzed in simple scenarios. Similarly, it was noted above that the scale of interest can sometimes be chosen so that it is only necessary to include a few key processes in the analysis. This will also generally decrease the number of types of boundary conditions that have to be

specified, and therefore, increases the isolation of the analysis from other scales. Still other boundary conditions, particularly the internal sources, can be tentatively specified even before any of the relationships are well understood. These arbitrary or decision boundary conditions can be developed in terms of the desired features of a repository. For instance, if it is expected or required that the repository will not raise temperatures more than 200°C above the ambient, that temperature can be specified as the temperature of rooms in a repository scale analysis. Just how the temperature is limited to that value need not be decided until a better understanding of the system is developed.

Generally, these relatively isolated analyses and simple models are the kinds of questions and assumptions to which analysis will be restricted in the very short term. Because of current limits on modeling capabilities, data, and budgets, models at both the repository and room scales will be able to include only moderate to low levels of detail. Because of this coarse detail throughout, the models used simply will not be able to assimilate or include detailed information about smaller scale phenomena into the specification of their necessarily coarsely sketched boundaries. This is not to say that such added information will not be useful in developing the effective values on which boundaries will be based. Detailed information will ultimately help in understanding the system. However, modeling of repository systems is a field which is only beginning to be developed. Boundary conditions that are simple relative to the actual complexity of the system are all that can be integrated into the mathematical analyses at this time. For example, currently the

capability to analyze a repository at the mine scale is limited to relatively coarse detail or very simple repository structures. Specification of the internal boundary conditions (or source terms) in repository scale analyses may at present be properly based on large scale average properties with assurance that the analysis will be consistent within the level of detail included. These large-scale averages can be postulated, regulated, or estimated without first solving the room scale analysis in its entirety.

In the short term, we are optimistic in general about the prospects for the success of analyses of repository performance with the most difficult problems foreseen in the application of the decomposition modeling approach being the coordination of the room and mine scales. We expect intermediate scale analyses to be manageable with little coordination to the smaller scales. Much less simple will be accurate specification of external boundaries for models at the room scale. In order to insure meaningful results, the boundaries will generally need to be located somewhere outside the convenient size for modeling the room scale (too many rooms included) and at locations that require a mine scale analysis at an inconvenient level of detail to specify boundary values. By "inconvenient", we mean that in order to place the boundaries at locations at which undisturbed values of system properties may be specified, a simple question concerning the performance of a design feature in one room may require modeling a number of rooms. The more rooms that have to be included in the analysis, the more unwanted and, for the most part, unproductive computational burden will be involved in the room scale

analysis. At the same time, if the mine scale analysis is restricted (in order to estimate accurate boundary conditions for a room

scale model) to a level of detail in which individual rooms have to be included in the analysis of the entire repository, the capability of current hardware and numerical model codes will be severely strained. Both the primary and secondary analyses will be difficult for practical reasons.

As noted above, progress toward an analysis of the entire repository system through the convention of analyzing the processes at each of the scales in light of relationships to the other scales, may be begun immediately by studying scenarios that can be isolated in terms of individual scales and may productively proceed through a gradual increase in the complexity of the scale relationships included in the analyses. At the same time, the complexity of details that can be included in analyses and the specificity of questions to be answered will be increased. This progress will be achieved in general through the increasing understanding of repository systems developed through experience with the simpler analyses, in particular through development and specialization of methods of analysis of particular aspects of repository performance, through posing better questions or the same questions in more manageable terms, through expansion of numerical hardware and software capabilities and efficiency, and through the development of reliable data bases.

II. SURVEY OF REPOSITORY SCALE CALCULATIONS OF NUCLEAR WASTE REPOSITORY HYDROLOGY

The decomposition modeling approach proposed in the last chapter is a response to the limitations that we perceive in experience with and capabilities for carrying out meaningful analyses of repository hydrology and a response to the pressing needs of the NRC. The limitations include meager data bases and limited understanding regarding the processes that will control repository performance. Also included are the very real difficulties in application of numerical methods to problem statements at the level of detail required in these analyses. The decomposition approach should allow immediate and continuing strides to be made in the analysis of repository performance within these limitations now and in the future as the limitations are forced back through research.

In order to determine what these technical limitations are, a survey of researchers in the field was funded by LLL and performed by New Millennium Associates (Holland and Wilson, 1979). The survey consisted of discussions with representatives of nine research groups around the country that have been involved in studies of waste migration and groundwater flow. This chapter is a summary of the results of that survey. All quotes are from the NMA report unless otherwise noted.

Discussions with the Research Community

During the course of the survey, the following facilities were visited and personnel contacted by staff members of New Millennium Associates:

1. Rockwell Hanford Operations, Richland, Washington; R. C. Arnett.

2. Battelle Pacific Northwest Laboratory, Richland, Washington;
John Raymond, et al.
3. Electric Power Research Institute, Palo Alto, California;
Robert F. Williams.
4. Stanford University, Department of Geology, Palo Alto, California;
Konrad B Krauskopf.
5. Lawrence Berkeley Laboratory, Berkeley, California; Chin-Fu Tsang.
6. Office of Nuclear Waste Isolation, Battelle Institute, Columbus,
Ohio; James O. Duguid.
7. Princeton University, Department of Civil Engineers, Princeton,
New Jersey; George Pinder.
8. United States Geological Survey, Reston, Virginia; J. Robertson
and Peter Stevens.
9. Sandia Corp., Albuquerque, New Mexico; James Cambell.

As a result of discussions with the various workers, the following general conclusions were drawn:

"In a word, our conclusion is that no one has yet formulated models nor performed calculations of the kind that we had originally envisaged and discussed with members of LLL. Some workers evinced an interest in the problem, and indicated an intent to address it in the future. Others were of the opinion that their codes could be adapted to solution of the repository flow problem, but saw no compelling reason to perform such detailed calculations, at least not at present. Still others have actually performed calculations on some aspects of the problem, but have not attacked the problem in its entirety".

In the following paragraphs, an abstract of the pertinent results of each of these discussions will be presented.

Rockwell Hanford Operations (RHO)

The RHO has been involved in applications oriented work in nearly all aspects of nuclear waste management. The complex has a newly formed study group which is just beginning to study the repository scale problem. Work in this regard is still very much conceptual in nature.

R. C. Arnett was the worker contacted at the RHO complex. Arnett suggested, to quote the NMA report,

"that among the potentially important effects for the near-field problem are hydrologic, thermal, chemical reaction, and migration effects".

He also suggested that the results of near-scale models may find an important use as source terms for far-field regional models. Finally, Arnett feels that analytic modeling of near-field effects should be employed wherever possible to aid and/or test computer models.

Battelle Pacific Northwest Laboratories (PNL)

The PNL hydrology and waste migration group is a very competent team that has been involved in research and development in the general field for some fifteen years.

The contacts at Battelle were J. R. Raymond, C. R. Cole, and A. E. Reisenaur. It was NMA's impression that although the work of these personnel and others at PNL may find applications in near-field analyses, work in this field has only recently begun.

The PNL effort, in general, includes several analytic and/or numerical models, some of which are coupled together, and all of which are isothermal. These programs include a pleasing degree of operator interaction

and graphics capabilities. The system attempts to make full use of the analyst's intuition as to system behavior. The PNL also has a waste migration model called Discrete Particle Random Walk (DPRW) which includes advection, dispersion, and radioactive decay. The algorithm is recommended by its outstanding numerical accuracy in dealing with the transport equation.

The PNL group feels that the large and increasing array of analytical and numerical systems in use in the nuclear waste isolation research community suggest the need for a general evaluation of the various systems by a group not involved in model development. In this way, redundant efforts could be identified, evaluated, and if necessary, redirected. We might interject at this point that no such proliferation of models for repository scale analyses exists, since very little work has been done in this field to date. Since many of the models developed for larger scale analyses may be adapted for use in the near-field, this proliferation may work to our advantage initially by allowing a wide range of models and codes to choose from.

Electric Power Research Institute (EPRI)

The Electric Power Research Institute has a small five-man. level of effort program studying nuclear waste disposal. The institute also funds work by Science Applications, Inc., and the The Analytic Science Corporation (TASC).

Part of the TASC work has involved analytical and simple numerical modeling of flow and transport near and through the repository. These

analyses are based on the very simple "box and shaft" models of the repository at what is called the repository scale in our hierarchy of length scales.

According to NMA's contact, Robert F. Williams, EPRI is basically interested in providing,

"an illustration of feasible waste disposal technology, an example of prospective criteria, and a comprehensive perspective to the public on the U.S. program, drawing upon the much larger efforts of the DOE, the NRC, and the EPA" (Williams, 1979).

As such, their work has concentrated on risk assessment analyses at all scales.

Williams has stated the belief that in many cases large R&D efforts may be avoided by concentrating on engineering solutions that ameliorate the need for detailed mathematical studies. He has expressed a particular concern about thermal effects in this regard.

Lawrence Berkeley Laboratory (LBL)

A group at LBL has been extensively involved in nuclear waste isolation analyses. The group is headed by Paul A. Witherspoon. NMA's contact at LBL, Chin-Fu Tsang, is involved in the modeling efforts of this group.

LBL is involved in extensive studies of fractures and fracture flow. The group is involved in field studies at the Stripa Mine site in Sweden, and in the Climax Stock experiment. The LBL group hopes to use the information gained in these studies to develop methods of constructing three-dimensional representations of fracture networks.

Tsang believes that modeling tools,

"exist which could be applied to the near-field repository problem, but that the running time would be very long".

Tsang also believes, and this seems to be the stance of the LBL group, that,

"it is not worthwhile to attempt to model near-field effects until these uncertainties (concerning fracture flow, sorption, and chemical effects) are cleared up".

Office of Nuclear Waste Isolation (ONWI), Battelle-Columbus

Battelle-Columbus operates ONWI for the Department of Energy.

James O. Duguid was the contact at ONWI. NMA reports that:

"Duguid thinks that the near-field repository problem is very important and that there presently exist no codes and/or programs which address this problem in a way consistent with its importance. ONWI is in the process of negotiating a substantial contract in this area (contractor unspecified). Duguid believes that analytic, as well as numeric modeling is required for an appropriate treatment of the near-field problem".

Duguid also identified the lack of adequate thermal-mechanical models as a problem area in repository scale analyses.

Princeton University, Department of Civil Engineering

The contact at Princeton University was Professor George F. Pinder, a well known name in the field of numerical groundwater transport and flow models as well as groundwater analyses in general.

Pinder said that,

"in a sense, one may consider the near- and far-field problems to be solved".

NMA's impression of his position is that he believes that the numerical models available are sufficiently general to solve repository problems as well as they can be solved in view of the limitation in the site data.

Pinder draws this conclusion, in part, on the basis of the Princeton group's past work for Sandia Laboratories on modeling mass transport and groundwater flow under conditions of data and parameter uncertainty.

Pinder's group collection of numerical models include three-dimensional finite element mass transport codes, fracture flow plus porous-medium flow models with mass transport, and a geothermal steam and water flow code.

United States Geological Survey (USGS)

The USGS has several numerical hydrologic codes which they have used in studies of repositories at regional scales. The Survey has not been involved in, and does not appear to be planning to carry out near-field repository studies.

John B. Robertson of the USGS believes, however, that,

"some one of these codes, or perhaps several used in conjunction, could be employed in near-field repository flow calculations".

The USGS has been involved in extensive studies of geothermally fractured igneous rock and of the fractured sedimentary rock overlying these members. This and other USGS work addresses fracture-flow and thermal (mostly thermal-mechanical) effects both locally and regionally, and thus may be helpful in future repository performance analyses.

Peter Stevens, whose work relates to the rock mechanics of repositories, expresses the opinion that,

"the near-field effects are important; in particular, thermal effects, rock mechanics, hydrology, and waste transport".

Stevens is involved in reviewing heater experiments, spent fuel experiments, etc., for the Earth Science Technical Plan for Mined Geologic Disposal of Radioactive Waste, a joint USGS and ONWI project.

Sandia Laboratories

To quote the NMA report,

"the Fuel Cycle Risk Analysis Division of Sandia is funded by NRC to develop a methodology for assessment of the long-term risks from disposal of radioactive wastes in deep geologic media. The analytical methods and data developed in the study are expected to form the basis for a portion of the NRC repository licensing procedure".

Sandia's primary analytical tool for hydrologic analyses is the Sandia Waste Isolation Flow and Transport code, SWIFT. A version of this same code is available to LLL. The code was developed for Sandia by Intera Corporation, a modification of Intercomp's SWIP code (also developed by Intera Corp.). The SWIFT code includes heat conduction, advection and convection, as well as groundwater flow, mass transport, and radioactive decay in two- and three-dimensions.

Currently, Sandia is only involved in regional scale studies, but James E. Campbell, NMA's contact there, believes that,

"SWIFT could be used for detailed near-field calculations, but that machine storage would quickly become a problem. Indeed, they are already storage limited in the regional calculations on the CDC 6600 they are presently using".

He also suggests, however, that even if machine storage were not a consideration,

"one runs the risk of being smothered with output, while failing to gain real understanding of the problem".

He favors instead,

"the formulation of rather simple models to be used for a number of exploratory calculations. These permit one to develop an intuitive feel for the problem, and provide a basis for determining which effects and parameters are important, and how the various phenomena are coupled".

Sandia also works with simple repository performance models employing the DYNAMO code, and is developing simple pipe flow models of repositories to be calibrated against SWIFT.

Conclusions

The viewpoints collected by NMA in their survey of workers in the field of nuclear waste management vary considerably in tone. Several, such as the LBL group and Dr. Krauskopf of Stanford, were pessimistic about the prospects for numerical modeling of near-scale hydrology and radionuclide transport. Others, such as the Sandia group, were more optimistic although still rather guardedly so. NMA reached some rather general conclusions through this survey. These conclusions will be presented below, followed by a brief discussion of points raised in the discussions as they apply to the proposed decomposition approach.

NMA concludes their report with the comments,

"Everyone we contacted in our survey believed the near-field flow problem to be an important one, and one that has not been adequately studied up to the present time. All agreed that, in principle at least, the flow problem comprises many complex,

coupled phenomena. These include dissolution, sorption, chemical reactions, thermal fracture, fracture flow, convection, heat conduction, etc., and the temperature dependence of various rate constants and equilibrium constants. Not only are these phenomena and their interrelationships not well understood per se, but the data base required for quantitative studies is also sadly deficient".

They also identify two proposed approaches to the investigation of near-scale repository analyses. The first approach suggests that before direct mathematical analyses of the repository are attempted, extensive measurement and data gathering programs should be conducted. Analysis in the absence of a firm data base, this approach suggests, will lead to very little useful information. The second approach suggests that the initial effort should consist of analyses and parametric (or generic) studies to determine which processes are important, which parameters must be determined, and to what degree of certainty they must be determined. The results of these studies will help to guide the subsequent data development program and insure that it is efficient.

NMA suggests that a course in which these two approaches are pursued con-
currently may be the optimal program.

Discussion of the Survey Results in Light of the Proposed Decomposition Approach

As noted above, the scarcity of data that so many of the modelers are concerned with is not a convincing reason not to develop and apply analysis methods to generic repositories. Analyses can be made that will help identify data needs. On the other hand, one cannot deny the limits on the data base that current analyses must rely on. Therefore, we must

agree with NMA's conclusion that the first step in developing or understanding of the "near-scale" repository system and repository performance in general should be a parallel drive to develop the basic data on which future analyses can be based and to perform parametric and generic analysis which will serve to direct future measurement programs. We believe the decomposition approach to modeling repository performance is a reasonable and efficient approach to follow in carrying out the second of these two goals.

The decomposition approach should allow us to begin this first step immediately. Thus, determinations of data and analytical needs can begin to be outlined in a very short time. At the same time, we believe that these same initial analysis can be employed in achieving tentative answers to some of the NRC's pressing questions. As noted in the last chapter, we expect the decomposition approach to prove productive almost immediately within the narrow range of the initial analysis.

The decomposition approach offers a framework for organizing and developing models of near-scale phenomena as they are developed. The proliferation of models pointed out by the PNL group is a problem chiefly because of the redundancies in the efforts of workers.

The survey has convinced us that very few models of the near-scale phenomena have been developed to date. A consistent overall modeling approach such as the decomposition approach is essential now for identification of the data needs and the modeling needs. Progress toward

answers within the decomposition approach should be fairly well determined by the logic of the approach itself. Thus, specific needs can be recognized and redundancies avoided.

Finally, the division of the repository performance problem into conceptually manageable sets (in this case, length scales) accomplished by the decomposition approach makes analysis very amenable to the development and use of the analyst's understanding and intuition about the system, such as advocated by the PNL group. The simplifications inherent in the choice of length scales allows a considerable portion of the analysis to be effectively discarded or performed before resorting to complex numerical models. At the same time, the approach encourages general understanding by maintaining a series of relatively simple models as opposed to a single enormous model. In this way the mountainous crush of output predicted by Campbell at Sandia is avoided. In general, the level of understanding of the system should be expected and encouraged to increase as the modeling program progresses. We believe that the decomposition approach will allow ample opportunity for this to occur.

III. PHYSICAL PROCESSES INVOLVED IN POST-SEALING REPOSITORY PERFORMANCE

In this appendix, seven important groups of physical processes in repository performance are discussed. The importance of these processes may be expected to vary considerably with the distance scale and scenario of interest. The processes are:

1. Advection transport.
2. Diffusion and dispersion.
3. Fracture flow/advection.
4. Dissolution and precipitation.
5. Sorption processes.
6. Thermal effects and processes.
7. Radioactive decay processes.

These processes will be described and the potential for modeling these processes in generic terms will be discussed below. These processes are discussed in more detail and the potential for parameterization of these processes for site specific analyses are discussed in "Processes and Parameters Involved in Modeling Radionuclide Transport from Bedded Salt Repositories," (Evenson, et al, 1979). Although that report is primarily concerned with regional scale transport, the discussion is wide-ranging and may be used as a reference for analysis within our hierarchy of scales as well.

Advective Transport

Freeze and Cherry (1979) define advection as "the process by which solutes are transported by the bulk motion of flowing groundwater," that

is, solutes dissolved in a fluid will be carried along with the fluid as it flows.

Mathematically, the rate of advective transport under steady flow conditions can be expressed as:

$$m = uc$$

where

m = rate of advective transport in terms of mass transported per unit time through a unit area (gm/sec/cm^2)

u = seepage or average pore velocity (cm/sec)

c = concentration of the solute (gm/cm^3)

The seepage velocity is the average rate of fluid flow through the pores in a porous medium. It is related to the apparent velocity, the average rate of fluid flow per gross area (pores and solid matrix) in the porous medium, by

$$v = un$$

where

v = apparent velocity (cm/sec)

n = effective porosity (fractional)

In most porous media, the apparent velocity is given by Darcy's Law:

$$\vec{v} = -\frac{k}{\mu} \left[\nabla \phi + \frac{\rho - \rho_0}{\rho_0} \nabla Z \right] = -\frac{K}{\rho} \left[\nabla \phi + \frac{\rho - \rho_0}{\rho} \nabla Z \right]$$

where

k = specific permeability tensor (cm^2)

K = hydraulic conductivity (cm/sec)

∇ = gradient operator

γ = specific weight of the fluid = γ (dynes/cm^3)

ρ = density of the fluid (gm/cm^3)

ρ_0 = a reference density (gm/cm^3)

g = acceleration of gravity (cm/sec^2)

μ = viscosity (poises)

ϕ = piezometric head, a measure of the pressure and potential energy at a point in the porous medium (cm)

Z = vertical distance from an arbitrary datum (cm)

The head distribution must be known if v and the resulting advective transport are to be predicted. This distribution is generally calculated by combining Darcy's Law with the equation of continuity, which is expressed:

$$n \frac{\partial \phi}{\partial t} = -\nabla \cdot (\rho v)$$

where t represents time. The results of combining the equations, in their three dimensional form, is the equation:

$$S_s \frac{\partial \phi}{\partial t} = \nabla \cdot \left[\rho K \left(\nabla \phi + \frac{\rho - \rho_0}{\rho_0} \nabla Z \right) \right]$$

where

S_s = storage coefficient, defined by

$$n \frac{\partial \rho}{\partial t} = S_s \frac{\partial \phi}{\partial t}$$

Under most conditions, this equation is a linear differential equation in terms of the unknown piezometric head distribution. Given an appropriate set of boundary conditions, it can be solved. Once ϕ is known, $\bar{v}$ and the resulting advective transport can be directly calculated.

It is not yet clear whether flow through salt can be described by Darcy's Law, particularly in situ. Until a valid description of fluid flow through salt is obtained, two methods of modeling advection through such media have been suggested by modelers. The first is to assume that in fact, Darcy's Law does apply. Under this assumption, a number of values for the specific permeability of salt have been obtained through laboratory measurements, ranging from 4×10^{-11} to $6 \times 10^{-24} \text{ cm}^2$ (Evenson, et al, 1979). These are very small values compared to most aquifer materials and thus salt is nearly impermeable. One argument for this first approach to modeling flow through salt is that with such low permeabilities, little flow will pass through the salt in any case and so the error in applying Darcy's Law will be small. This approach is somewhat more conservative in terms of modeling potential radionuclide transport than the second suggested approach which is to assume that the salt media are strictly impermeable. There is no fluid flow in an impermeable medium, and where there is no fluid flow, there can be no advection. Thus under this assumption, there is absolutely no advective transport through the salt. Given the small values of permeability obtained in laboratory measurements and the ability of salt, through plastic deformation, to heal any fracture openings, it is expected that in situ salt will act under most circumstances as a very good barrier to

flow. The problems that plague this second approach are primarily a result of the long time scales involved in models of nuclear waste repositories. Although over short time periods, such as those encountered in laboratory measurements, salt appears to be very nearly impermeable; there is no good data on the potential for flow within a salt member over the time spans of interest. Therefore, any model of fluid flow through salts is bound to be primarily speculative.

The importance of the question of whether salt is impermeable or not will depend on the distance scale and the scenario that one is concerned with. At the room scale, the importance of flow through salt will often be minimal. Because it is difficult to imagine a material which could be used to backfill the repository structure which would be less permeable than the surrounding salt, it is likely that more fluid flow will take place within the repository than in the salt. Thus, advection within the repository will tend to dominate advective transport through the salt. In some scenarios it is possible at the room scale for advection through salt to be important because, although such advection would be very slow (since the permeability is so low), the distances that advected radionuclides have to travel to be of interest are also rather small. For example, when an impermeable plug in a corridor is hypothesized, advection through the salt around the plug may be important. At the repository scale, in most cases it is expected that flow through the repository itself will be more important than flow through salt. The distances that radionuclides would have to be advected to be noticeable at this scale of discretization (detail) and the corresponding travel times are so long

that it is expected that other radionuclide escape scenarios will be more important than simple advection through salt. Finally, at the intermediate distance scale, advection through salt will generally be so slow as to be unimportant except after very long times. An exception to this generality is the case where the presence of large-scale fractures or discontinuities in salt beds greatly increase the "apparent" permeability of the salt bed. This exception will be expanded upon when fracture flow is discussed below.

Diffusion and Dispersion

Diffusion and dispersion are processes that irreversibly distribute solutes within porous media.

The term diffusion is often used in reference to molecular diffusion, a physiochemical mixing process resulting from chemical potential gradients where solute concentrations are variable. Temperature and pressure gradients may also serve as driving forces for the diffusion process. In a homogeneous porous medium, the diffusion process is described mathematically as:

$$\frac{\partial c}{\partial t} = D' \nabla^2 c$$

where

D' = porous medium diffusion coefficient (cm^2/sec) (Fried and Combarnous, 1971).

Dispersion, on the other hand, is a general term describing mixing brought about by the vast number of complex flow paths along which constituents are carried as the solute is advected through a porous

medium. Differences in flow path length, flow velocity, and travel times result in longitudinal and lateral mixing which is referred to as dispersion. This process ranges from the microscopic scale mixing brought about by the extraordinarily convoluted geometries of pores within a porous medium to the regional scale process, macrodispersion. Macrodispersion refers to the mixing induced as a solute is transported across the large-scale permeability heterogeneities in most large aquifer systems. Dispersion is included mathematically in the advection-dispersion equation:

$$\frac{\partial C}{\partial t} + \nabla \cdot (uC) = \nabla \cdot [\underline{D} \cdot \nabla C]$$

with

u = seepage velocity (cm/sec), and

$\underline{D}$ = dispersion coefficient tensor (cm²/sec).

Dispersion and advection are intimately related and one is never seen without the other. The form that the dispersive component (the right hand side) takes in this equation was chosen in direct analogy to the diffusion equation above. At the regional scale, this analogy becomes questionable in many aquifers, and the equation as presented is suspect. This problem is discussed in considerable detail in "Dispersive Processes in Models of Regional Radionuclide Migration," prepared for LLL by Camp, Dresser & McKee (Evenson and Dettinger, 1980).

The diffusion coefficient D' ranges from 10^{-5} to 10^{-8} cm/sec (Lerman, 1971) while the dispersion coefficient is often formulated as

$$D = \alpha u$$

where

α = the dispersivity (cm).

The dispersivity ranges in values from millimeters for small-scale systems (on the order of one meter), to tens and hundreds of meters in field systems (on the order of 100-1000 meters).

Fracture Flow and Advection Through Fractures

Fractures, whether naturally occurring or opened during construction of the repository, represent an important pathway for the transport of radionuclides from the repository to surrounding aquifers. Fractures tend to act as pipes through which contaminated fluids may pass with little resistance compared to the Darcian flow law. Thus, potentials for fracture flow must be assessed, and if necessary, incorporated into models of repository performance.

The flow through a single fracture may, under numerous simplifying assumptions, be approximated by equations such as:

$$q = \frac{(b)^3}{12\mu} \rho g \frac{\partial \phi}{\partial x}$$

where

q = the discharge per unit width of fracture (cm^2/sec)

b = fracture aperture (cm)

ρ = fluid density (gm/cm)

μ = viscosity (poises)

ϕ = piezometric head (cm)

x = distance along the fracture (cm).

This equation describes non-turbulent flow of an incompressible Newtonian fluid between two parallel plates (Gale and Witherspoon, 1979).

Generally, where fractures are present, they are present in large numbers. In any case, fractures are difficult to enumerate and parameterize. This has lead several researchers, e.g., Witherspoon of LBL, to suggest complex probabilistic mathematical descriptions of the effects of fracture flow. At the opposite extreme from the parallel plate model above, A Darcian equivalent porous medium is assumed. This model is not very accurate unless the medium is highly fractured. It is presented here for the purposes of discussion. The model may be expressed as:

$$\mu = \frac{K_f}{n_f} \frac{\partial \phi}{\partial x}$$

where

K_f = the bulk hydraulic conductivity of the fractured medium

n_f = the bulk fracture porosity (Freeze and Cherry, 1979).

This equation is based on the assumption that the fractured medium acts very much like a porous medium when a large enough volume (including many

fractures) is analyzed. As noted above, flow through a fractured medium occurs mostly in the fractures and thus, it is the fracture void or porosity that is used in the above equation. The hydraulic conductivity will also be markedly different from the conductivity of the unfractured medium.

In salt, fracture flow/advection should be viewed from a different perspective. As noted earlier, salt through plastic deformation is able to heal most fractures, and therefore, it is expected that there will rarely be more than a few major fractures active at any scale. Fractures do, however, occur. Major fractures, if sufficiently extensive, may be kept open by dissolution or mechanical forces and would have to be handled individually (Carpenter, Steinborn, and Thorson, 1979). Bedded salts are also often interbedded with materials and strata of somewhat higher permeability than the surrounding salt. These interbeds may act as very efficient pathways for radionuclide transport. Such pathways can be included relatively easily in analyses if they are treated as permeable paths through an impermeable medium, that is, essentially the same way that fractures are dealt with. At the room and mine scales, the individual pathways or aggregates of the pathways will have to be dealt with individually and specified in terms of their length, orientation, and flow characteristics in the scenario statement. At the intermediate scale, there is the chance that sufficient interbedding will be included and that a large scale Darcian formulation may be applicable.

Dissolution and Precipitation

Dissolution is the process by which a solid is dissolved or broken

down into its ionic components in a liquid. Precipitation is the opposite of dissolution. Salts are very soluble and dissolution/precipitation can play an important role in altering the boundaries and flow properties in and near bedded salt and dome salt repositories. Fractures and other pathways, including corridors, through the salt can be enlarged or otherwise reshaped by dissolution of the surrounding salt into water flowing through them. At the same time, the fluid density and other flow properties may vary considerably as the amount of salt dissolved in the water increases (See Figure 2). If a repository located in salt is to be analyzed, dissolution will have to be accounted for.

The rates and volume of dissolution and precipitation depend on the degree of under- or over-saturation of the solvent with the solute and the surface area of the solute that is in contact with the solvent. The degree of saturation is equal to the concentration of solute in the solvent divided by the concentration at which dissolution and precipitation exactly balance. In the case of groundwater flow through salts, the rate of dissolution is fast, and the flow slow, so that the water is nearly always salt saturated (Clarborne and Gera, 1974). The saturated fluid does not dissolve additional salt, but between the time it enters the system as fresh water and the time that it reaches saturation, the amount of salt dissolved is

$$\left[\text{Solubility (mg/l)} \right] \times \left[\text{Volume of fluid (l)} \right] .$$

If this amount is substantial compared to the volumes of salt being analyzed for a particular distance scale and scenario then a means of including dissolution will have to be developed.

Figure 2. Density of the liquid phase for vapor-saturated NaCl solutions from 0 wt percent to halite saturation at 80° to 325° C. Contour interval is 5 wt percent NaCl. The shaded zone was calculated by extrapolating the functions given in the text (from Haas, 1976).

The solubility of salt is a function of temperature, pressure, and chemical composition. Of these parameters, chemical composition is most critical, and since salt beds vary considerably, solubilities will have to be determined at the site of interest. Temperature is also important since a broad range of temperatures are expected in the repository environment. As the fluid flows from one temperature regime to another, its degree of saturation will change and further dissolution or precipitation may take place. The range of pressures in the repository are expected to be such that pressure effects on solubility will be negligible.

Dissolution and precipitation change flow characteristics, boundary conditions and even the flow field as they progress. For these reasons, they are generally very difficult to include in mathematical analyses of

transport systems. Two approaches to modeling these processes present themselves; the first, a simple representation of their averaged effects, and the second, a complicated simulation of the entire processes. The simple approach is to model the effects of dissolution on the transport system solely in terms of variations of the flow properties and parameters. This might be accomplished by functionally linking bulk fracture porosities and permeabilities to the amount of fluid that has passed through the fractured regions, thus simply representing the overall increases in fracture apertures brought about by dissolution. This approach might also be applied to flow through single fractures. Generally, this approach would be very approximate and could only be applied where changes due to dissolution are not catastrophic. In cases where large-scale changes to the repository system result from extensive dissolution, as in breccia pipe formation, prediction of repository performance will require models of dissolution of considerable detail. In such instances, the highly nonlinear problem of predicting how much the boundary locations have been altered, along with the effects of these changes, will have to be solved. Techniques do exist for solving related problems such as locating the boundaries of melting icecubes in water (Sa DaCosta, 1979) but considerable study would be required to adapt existing mass transport codes to this purpose.

Sorption Processes

Sorption processes are primarily chemical in nature and include adsorption, ion exchange, colloid filtration, reversible precipitation, and irreversible mineralization (Burkholder, 1976, and Burkholder, et al,

1975). The first two processes are most important in repository performance and result in attenuation of radionuclide transport through porous media so that the radionuclides are transported more slowly than the bulk flow rate of the advecting water. Ion exchange and adsorption are processes which involve the temporary binding of radionuclides to the surface of the solid matrix of the porous medium (Evenson, et al, 1979).

Sorption processes are generally very complicated and are described by a large variety of parameters. Of immediate concern is the sorption equilibrium constant γ which allows sorption to be included through a simple alteration of the advection-dispersion equation for transport of the radionuclide through the medium. The equation becomes (Gershon and Nir, 1969):

$$\frac{\partial c}{\partial t} = \frac{D}{\gamma} \nabla^2 c - \frac{u}{\gamma} \nabla c$$

where

D = dispersion coefficient (cm^2/sec)

u = seepage velocity (cm/sec), and

γ = sorption equilibrium constant

under equilibrium conditions and when there is little competition between chemical species. The sorption equilibrium constant can be calculated on the basis of the stoichiometric relationship describing the chemical interaction, the mass-action equilibrium constant for the reaction, the concentrations of the solute being sorbed in the fluid, and on the solid matrix, the porosity and the density of the porous medium. The coefficient is given in general terms by (Lai and Jurinak, 1972):

$$Y = \frac{1}{n} \frac{\partial c_s}{\partial c} + 1$$

where

c_s = mass of radionuclides sorbed per volume of porous medium (mg/l)

c = concentration of radionuclides in water (mg/l)

n = porosity

Often $\frac{\partial c_s}{\partial c}$ is assumed to be a constant and a distribution coefficient K defined equal to that ratio. The distribution coefficient is, conceptually, the "amount of the subject ion sorbed per gram of solid, divided by the amount of ion in solution per cubic centimeter of liquid after equilibrium is achieved" (Borg, et al, 1976).

Under most circumstances, it is anticipated that sorption processes will reach equilibrium more quickly than the radionuclides that are transported, and the above simple correction to the transport equation may be applied. Sorption during flow through fractures may be an important exception to this generality since the surface area sorbed to is relatively small and flow velocities large (Freeze, 1979). Another exception might be at the room scale where distances and travel times are small. At this scale, equilibrium might not be reached as transport progresses and nonequilibrium sorption would have to be modeled. The simplest and most common approach to nonequilibrium dynamics is to assume a linear reaction model (assuming sorbed constituents are a small fraction of the total):

$$\frac{\partial c_s}{\partial t} = -k_1 c$$

which results in the following adapted advection-dispersion equation (Gershon and Nir, 1969):

$$\frac{\partial C}{\partial t} = D \nabla^2 C - u \nabla C - k_1 C,$$

which is similar in form to the transport equation in the presence of radioactive decay. Solution of this equation is a relatively simple amendment to solutions of the original transport equation.

The techniques for including sorption processes in radionuclide transport analyses are quite simple, and may well miss some of the finer details of the effects of these processes. At most scales, however, given the long travel times and the difficulties that will be involved in parameterizing any sorption models, we expect that the simpler the model is and the fewer parameters involved, the better will be the results.

Finally, it should be noted that sorption processes will have little or no effect in salt. The chemical nature of salts is such that the distribution coefficients are virtually zero. Therefore, sorption processes will be most important in the backfill material inside the repository structure and in porous materials encountered outside the salt members.

Thermal Effects and Processes

The heat generated as a result of high radionuclide concentrations in the waste canister buried beneath the floor of the repository leads to a wide variety of thermal effects that may have very important consequences in determining repository performance. Among these effects are changes to the material properties of the porous media that make up the repository,

the establishment of convection currents, and thermomigration. In the following paragraphs, the nature and potential importance of a number of these effects will be discussed.

The three important means by which heat is distributed within a porous medium may be described as conduction, forced convection, and free convection. Conductive heat transfer refers in this context to heat transfer between parts of the medium that are in direct contact. Heat may be expected to be transferred by conduction through the solid matrix, through the fluid, and between the solid and fluid. Conduction is not a very effective means of distributing heat compared to the others, but in cases where fluid flow is negligible due to low permeabilities, etc., conduction will dominate. In salts, this process will have to be accounted for very carefully and over long distances. Forced convection is a term that describes the transport of water from a region at one temperature to another region that is either warmer or cooler. Forced convection is caused by an externally imposed flow field; that is, the temperature gradients are not the driving force for the flow. Forced convection may be described as advection of heat. Although the density of the fluid as well as other properties are expected to be affected by temperature, this sort of advection is exactly analogous to the advection of radio-nuclides discussed above. There will also be a thermal macrodispersion effect. Free convection, on the other hand, is the movement of heat and fluid arising as a result of currents driven by the heat source itself. The driving mechanism is buoyancy resulting from variations in fluid density arising from temperature variations in the fluid. Convection,

in general, is limited by the amount of fluid that can be moved through the medium. Also important are the temperature gradients which drive convection (Combarrous and Bories, 1975). In low permeability salts, flow is severely limited, and thus convection will often be negligible. This suggests that convection will be important at the repository scale within the repository rooms and corridors where the permeabilities may allow some flows and the gradients may be developed to a sufficient degree.

Modeling these different forms of heat transfer requires different mathematical capabilities. Conduction is relatively easily assessed and a large variety of analytical (Carslaw and Jaeger, 1959) and numerical methods and solutions (Chan, et al, 1978) are available. Forced convection is simulated in exactly the same manner as solute advection with the exception that flow and transport processes are functions of the temperature. It is therefore a nonlinear problem, but is only mildly nonlinear and mildly difficult unless very large differences in temperature are encountered within the problem boundaries. Free convection is a highly nonlinear problem in which density variations induced by heating drive the flow which distributes the heat. Because of this high degree of nonlinearity, solutions will be relatively expensive and obtained only as a result of some very complex computations.

It is important that any thermal model of a repository have the capability to simulate all three of these processes, unless one of them is definitely known to be negligible. A calculation of temperatures that fails to

model any one of these processes will provide useless results if that one is of importance comparable to the others. This is because the effects of each is completely different from the others. Conduction produces smoothly varying temperature profiles while forced convection generates temperature profiles that vary as rapidly as the flow field. On the other hand, within a uniform flow regime, forced advection will minimize the temperature gradients and temperatures while free convection leads to flow cells that show large variations in temperature.

A number of approximations may be applied in solving the above heat transfer problems. A very common approximation in developing models of these heat transfer processes is Boussinesq's approximation. Under this approximation, it is assumed that "variations in fluid density are negligible except in the buoyancy term" (Combarrous and Bories, 1975). This should be acceptable for most temperature profiles encountered in repository systems and offers a considerable simplification to the governing equations. Another simplifying assumption that the solid matrix is always at thermal equilibrium with the fluid it encloses. This eliminates the need for inclusion of conduction between solid and fluid in the analysis. The assumption is justified unless the seepage velocities encountered are very large. The thermal properties of the porous medium, such as specific heats, are often assumed to be constant, resulting in only a small loss in accuracy. Finally, the viscous dissipation (kinetic energy) and potential energy of the flow are assumed to be negligible in comparison to the energy being transferred as heat (Garg and Pritchett, 1977). For a readable development of the equations

governing the temperature in a porous medium, see the development presented by Faust and Mercer (1979) in their treatment of geothermal systems. The resulting equations are almost exactly those presented by the documentation of the SWIFT model, a transport model with thermal effects adapted especially to the repository problem, but the description is more informative.

Finally, it is very important to reiterate that free convection is potentially very important to repository performance. The current set up by this process will tend to lift large quantities of water and perhaps radionuclides up out of the repository through any and all available pathways. It will generally increase the dispersal of the radionuclides as it develops. This process must definitely be understood if repository performance is to be accurately predicted.

Material properties of the porous media that make up the repository can vary considerably with temperature. Fluid density, viscosity, chemical properties, and even molecular diffusion are affected by temperature changes as well as mechanical properties of the solid matrix. If the variation of temperature within the region of interest is large enough at any of the scales so that the variation of any or all of these properties is important, the variations will have to be included in the models. Inclusion of these property changes should proceed, however, in full cognizance of and consistency with any use of the Boussinesq approximation in prior model development.

Changes in the mechanical properties of the solid matrix such as expansion induced by temperature changes, may prove very important in altering the boundary conditions for transport through the repository. Large and small fracturing as a result of such changes is a very definite possibility and threat to the integrity of the repository. Modeling of these complicated effects poses a difficult challenge to the modeling techniques available, since, in addition to being complex when isolated, they are in this case intimately related with the fluid flow and heat transport system of the repository. Generally, one would hope that thermomechanical effects could be minimized by measures such as regulating the areal heat loading and civil design of the repository. The means by which such regulatory methods and designs could be developed is outside the scope of this scoping study, but its success will have important consequences in determining how complex the modeling program will be. Models of these effects will have to be integrated into or with flow and heat transport models if the full extent of thermal effects on repository performance are to be assessed. Given the current state-of-the-art in modeling, such dramatic increases in the complexity of the repository performance problem are hardly called for.

Yet another potentially important thermal effect in salt is thermomigration. As stated by Cohen (1977), "The solubility of salt in water increases with temperature, so that if the temperature on one side of [a brine inclusion] is raised, more salt will go into solution on that side. This raises the salt content of the water above the saturation point for the temperature on the opposite side of the pocket, however, causing the

salt to precipitate out of solution on that side. The net effect is a migration of the water pocket in the direction of the higher temperature". At very high temperatures, biphasic stream-brine droplets or inclusions may be formed which tend to thermomigrate away from the heat source. According to Anthony and Cline (1974), neglecting droplet entrapment on grain boundaries, the temperature gradients expected in repository settings will lead to thermomigration of stream-brine droplets and perhaps radionuclides to distances of six meters or less in two years. Over geologic time, the total dispersal of radionuclides will not be noticeably increased by thermomigration, but in some room-scale scenarios the process may be of some importance.

Radioactive Decay Processes

Radioactive decay of radionuclides is a natural mechanism for the attenuation of radionuclide transport. The effect of radioactive decay on the concentration of radionuclides is given by the following equation (Evenson, et al, 1979):

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

where

$$\lambda = \text{decay rate constant (sec}^{-1}\text{)}$$

$$= \frac{0.693}{t_{1/2}}$$

$$t_{1/2} = \text{radionuclide half-life}$$

Notice that this process always acts to decrease the concentration.

Radioactive decay is an irreversible process which may, however, lead to

the generation of new (or daughter) radionuclides which are also hazardous. It is necessary then to include radioactive decay and creation calculations for all important "parent" and "daughter" radionuclides. This may be handled by keeping track of travel times of particles as they are transported and using that information to compute the amount of decay. As an alternative, explicit inclusion of the process in the solution scheme is not an intractable task in most cases.

Conclusions

Generally, as noted above, advection will be the prime mover in transporting radionuclides through and from the repository. Other important processes such as dispersion, sorption and thermal effects are essentially second-order effects or represent what are hopefully minor alterations to the advecting flow field. As a result, radionuclide transport models will have as a basis, some sort of advection model.

Dispersion and sorption are generally expected to effect radionuclide transport and repository performance, and therefore, should be modeled in most scenarios. Dispersion is included in nearly all available models of transport through porous media. Sorption is often missing from models but can in principle, be included in transport models quite easily.

Thermal effects and processes resulting from the heat generated by the waste forms have the potential of being very important. If conditions are such that free convection develops, then the entire advecting flow field may be changed. Under such conditions, flow through the repository would no longer be dependent on head differences produced by processes

external to the repository, but could proceed and vary independently from regional effects. Somewhat less important are the effects of temperature on flow and transport parameters which result in subtle changes to the advecting flow field or progress of radionuclide transport. Although we know that the potential influence of thermal processes may be quite important, our understanding of the repository system is such that no firm statement can be made regarding the actual or expected importance of these processes. Our acquisition of the capability to model thermal processes is important to the overall defensibility of the repository modeling program. Until a reasonable understanding of the role that these processes play in repository performance is developed, the value of modeling many scenarios will be limited.

The influence of the other processes: fracture flow, dissolution, and radioactive decay, will be very dependent on the particular scenario of interest. The scenarios under which they are important will generally be known before modeling begins. The particular medium being addressed and the discharge scenario that one is concerned with will, to a large extent, determine the importance of fracture flow/advection and dissolution, while the time period and travel times of interest will determine the influence of radioactive decay. Therefore, it appears that although the capability to model these processes should be developed, it will not be necessary in many analyses, and in fact, development of the capability can be regarded as an independent task to be motivated by the scenario of interest.

REFERENCES

Anthony, T. R., and H. E. Cline, "Thermomigration of Liquid Droplets in Salt," Proceedings of the Fourth International Symposium on Salt, Northern Ohio Geological Society Volume 1, 1974.

Borg, I. Y., et al, "Information Pertinent to the Migration of Radionuclides in Groundwater at Nevada Test Site, Part I: Review and Analysis of Existing Information," Lawrence Livermore Laboratory Report, UCRL-52078, 1976.

Burkholder, H. C., "Methods and Data for Predicting Nuclide Migration in Geologic Media," International Symposium on Management of Wastes from the LWR Fuel Cycle, Denver, BNWL-SA-5523, Battelle Pacific Northwest Laboratories, July, 1976.

Burkholder, H. C., M. O. Cloninger, D. A. Baker, and G. Jansen, "Incentives for Partitioning High-Level Waste," Battelle Pacific Northwest Laboratories, Richland, Washington, Rept. BNWL-1927 (11975).

Carnahan, C. L., "Nonequilibrium Thermodynamics of Groundwater Flow Systems: Symmetry Properties of Phenomenological Coefficients and Considerations of Hydrodynamic Dispersion," Journal of Hydrology 31, pp: 125-150, 1976.

Carpenter, D. W., T. L. Steinborn, and L. D. Thorson, "Groundwater Recharge and Discharge Scenarios for a Nuclear Waste Repository in Bedded Salt," Lawrence Livermore Laboratory Report, UCID-18119, March, 1979.

Carslaw, H. S., and J. C. Jaeger, Conduction of Heat in Solids, Oxford Books, 1959.

Char, T., N. G. W. Cook, and C. F. Tsang, "Theoretical Temperature Fields for the Stripa Heater Project," Swedish-American Cooperative Program on Radioactive Waste Storage in Mined Caverns in Crystalline Rock, LBL-7082 1/2, Technical Information Report No. 9, September, 1978.

Clarborne, H. C., and F. Gera, "Potential Containment Failure Mechanisms and Their Consequences at a Radioactive Waste Repository in Bedded Salt in New Mexico," Oak Ridge National Laboratory Report, ORNL-TM-4639, October, 1974.

Cohen, B. L., "The Disposal of Radioactive Wastes from Fission Reactors," Scientific American, Vol. 236 (6), June, 1977.

Combarous, M. A., and S. A. Bories, "Hydrothermal Convection in Saturated Porous Media," Advances in Hydro-Sciences, 1975.

Dames and Moore, "Groundwater Movement and Nuclide Transport," Technical Support for GEIS: Radioactive Waste Isolation in Geologic Formations, TM-36/21, April, 1978.

Evenson, D., T. Prickett, and P. Showalter, "Processes and Parameters Involved in Modeling Radionuclide Transport from Bedded Salt Repositories," Lawrence Livermore Laboratory Report, UCRL-15095, July, 1979.

Evenson, D. E., and M. D. Dettinger, "Dispersive Processes in Models of Regional Radionuclide Migration," for Lawrence Livermore Laboratory, Camp Dresser & McKee, Inc., March, 1980.

Faust, C. R., and J. W. Mercer, "Geothermal Reservoir Simulation, I. Mathematical Models for Liquid- and Vapor- Dominated Hydrothermal Systems," Water Resources Research 15 (1), pp. 23-30, 1979.

Freeze, R. A., and J. A. Cherry, Groundwater, Prentice-Hall, 1979.

Fried, J. J., and M. A. Combarous, "Dispersion in Porous Media," Advances in Hydrosiences, Vol. 7, 1971.

Gale, J. E., and P. A. Witherspoon, "An Approach to the Fracture Hydrology at Stripa: Preliminary Results," Swedish-American Cooperative Program on Radioactive Waste Storage in Mined Caverns in Crystalline Rock, LBL-7079, Technical Information Report No. 15, May, 1979.

Garg, S. K., and J. W. Prichett, "On Pressure-Work Viscous Dissipation and the Energy Balance Relation for Geothermal Reservoirs," Advances in Water Resources 1 (1), pp. 41-47, 1977.

Gershon, N. D., and A. Nir, "Effects of Boundary Conditions of Models on Tracer Distribution in Flow Through Porous Mediums," Water Resources Research 5 (4), pp. 830-839, 1969.

Haas, J. L., "Physical Properties of the Coexisting Phases and Thermochemical Properties of the H₂O Component in Boiling NaCl Solutions," U. S. Geological Survey Bulletin 1421-A, 1976.

Holland, D. H., and R. N. Wilson, "Analysis of the REPLO Hydraulic Model," Lawrence Livermore Laboratory Report, UCRL-15022, November, 1978.

Holland, D. H., and R. N. Wilson, "A Survey of Near-Field Flow Calculations for Nuclear Waste Repositories," Lawrence Livermore Laboratory Report, UCRL-15162, November, 1979.

Lai, S. H., and J. J. Jurinak, "Cation Absorption in One-Dimensional Flow Through Soils: A Numerical Solution," Water Resources Research 8 (1), pp. 99-107, 1972.

Lerman, A., "Time to Chemical Steady State in Lakes and Oceans," Non-equilibrium Systems in Natural Water Chemistry, Advances in Chemistry, Series 106, American Chemical Society, 1971.

National Research Council, "Implementation of Long-Term Environmental Radiation Standards: The Issue of Verification," National Academy of Sciences, Washington, D. C., 1979.

Sa DaCosta, A. A. G., and J. L. Wilson, "A Numerical Model of Seawater Intrusion in Aquifers," Ralph M. Parsons Laboratory for Water Resources and Hydrodynamics Technical Report No. 247, November, 1979.

U. S. Nuclear Regulatory Commission, "High-Level Radioactive Waste Management - Identification of Technical Support Requirements and Summary of FY80/81 Projects," The Office of Nuclear Material Safety and Safeguards, October, 23, 1979.

Williams, R. F., "Utility Programs and Approaches for Acceptable Radioactive Waste Management," Electrical Power Research Institute, September, 1979.