PERFORMANCE ASSESSMENT NATIONAL REVIEW GROUP

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A Report for Weston

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EXECUTIVE SUMMARY

The Performance Assessment National Review Group (PANRG) was established at the request of the U.S. Department of Energy's Office of Civilian Radioactive Waste Management (OCRWM) by Roy F. Weston, Inc. (Weston), the technical support contractor to the OCRWM. The convening of the PANRG was, to a considerable extent, in response to the recommendations of the Waste Isolation Systems Panel (WISP) of the National Research Council/National Academy of Sciences/National Academy of Engineering. In the WISP report, entitled A Study of the Isolation System for Geologic Disposal of Radioactive Wastes, it was concluded that performance assessment would be a key input in site selection and licensing of geologic repositories. The report recommended an overall technical review of performance assessment activities. Accordingly, the main objectives of the PANRG were to (1) carry out an independent review of the performance assessment work by the three Projects engaged in the selection and development of the first repository site and (2) provide recommendations as to how this work might be improved.

Performance assessment involves predicting the potential radiological impact of a nuclear waste disposal system, taking into account all of the natural and engineered components of the system. It includes the analysis and evaluation of predicted system and component performance to determine compliance with regulatory performance criteria. In the context of the nuclear waste management program mandated by the Nuclear Waste Policy Act of 1982 (P.L. 97-425), performance assessment has five major purposes—(1) to assist in the evaluation and selection of repository sites; (2) to guide the research, development, and testing programs; (3) to assist in the evaluation of repository designs; (4) to assist in the evaluation of the design and performance of engineered barriers; and (5) to show regulatory compliance and support repository licensing.

The PANRG carried out its review through two meetings with staffs of the salt, basalt, and tuff projects, at which presentations on specifically identified topics were given and discussed, and through several working meetings of the PANRG members. NRC staff participated in both briefings, and EPA staff participated in the first of the briefings with project personnel. The PANRG also had the benefit of discussions with OCRWM-Headquarters staff.

Observations and recommendations of the PANRG fall into two categories - (1) those related to management/institutional factors and (2) those of a technical nature. The former are presented in Chapter 2 and the latter in Chapter 3.

Management/Institutional Factors

- Scientists and engineers capable of carrying out the necessary performance assessments are available. Further needed experience should be developed as work progresses and as experience in working in licensing relationships with the Nuclear Regulatory Commission are developed more fully (see General Observation No. 1).

- Personnel and budget resources that have been allocated to performance assessment activities appear inadequate (see General Observation No. 2).

- Basic to these managerial/institutional observations and recommendations was the evident need for an integrated performance assessment plan. Such a plan should provide bases for defining both human resources and budgetary requirements and should identify communication mechanisms needed for better management of the overall performance assessment programs (see General Observation No. 2).

- The need for more coherent management of the performance assessment program was reflected in the apparently less-than-optimal level of communication between the Projects and Headquarters (see General Observation No. 3).

- The need for improved communications at all levels was evident. Within the Projects, closer working relationships between those making performance predictions and those gathering and analyzing data in the laboratory and the field are needed. Similarly, better communications at the project level will promote the exchange of ideas between Projects and the development of more effective solutions to problems of common concern (see General Observation No. 4).

- Of particular significance was the need for more effective working relationships between the Projects and the NRC in order to systematically identify and resolve licensing issues on a continuing, active basis (see General Observation No. 5).

- The PANRG recognized that, of necessity, the conduct of performance assessment is based in a fundamental way on the exercise of professional, technical judgment. These judgments should, therefore, be documented carefully, including their supporting rationale and logic (see General Observation No. 7).

- Although the proposed EPA standard and NRC regulations do not specifically require the calculation of radiation dose or risk, the PANRG believes that such calculational capability should be available in the Projects and that such calculations should be performed for time periods beyond 10,000 years (see General Observation No. 9).

<u>Technical Factors</u>

The PANRG's technical observations and recommendations address both
(a) the phenomenology and
(b) the methodology
involved in performance assessment.

Examples of the phenomenological aspects include:

- the current lack of adequate data on the characteristics of spent fuel, obviously the major waste form for the first repository, relevant to its behavior under potential repository conditions (see Technical Observations Nos. 5 and 6);

- the need for sufficient understanding of possible corrosion modes of waste canisters (see Technical Observations Nos. 4, 5, and 6 and Section 3.2.1);

- the importance of geochemistry in understanding the nature and behavior of the hydrogeologic system and in predicting radionuclide mobilization and migration was generally recognized by the Projects, but the need was apparent for more comprehensive and detailed investigations and better integration of the results of the investigations into systems analysis and evaluation (see Technical Observation No. 11); and

- the need to consider development of appropriate models to characterize the importance and role of the interactions and impacts of coupled phenomena (thermal, chemical, hydrologic, mechanical, and radiological) (see Technical Observation No. 12).

From a methodological standpoint, examples include:

- The need for developing defensible bases for the extrapolation of results from short-term experiments and tests to the long time periods required for postclosure performance assessment. For example, one alternative is to use a verifiable theory for predicting long term behavior that does not require extrapolation, such as mass transfer analysis (see Technical Observations No. 4 and 6).

- The desirability of more coordination in the handling of data uncertainties, including the incorporation of uncertainty analysis techniques into the various computer codes, and the application of techniques for sensitivity analysis in the guidance, direction, and setting of priorities for development and testing (see Technical Observations 8 and 9).

- The importance of probabilistic approaches to many aspects of performance prediction was generally recognized, but specific applications of probabilistic or stochastic techniques were not yet well defined nor were results of applications available from the Projects (see Technical Observation No. 8).

- Progress in the area of model verification and validation was indicated, but it was also evident that a more definitive, mutually accepted (with the NRC) operational definition of what constitutes validation is needed (see Technical Observation No. 7).

In summary, performance assessment is the major available tool to accomplish informed technical decisions and licensing of high-level nuclear waste repositories. Current performance assessment methodologies are still in the developmental stage. Only the simplest of bounding calculations have produced quantitative predictions of radionuclide releases. The methodologies require considerable extension and validation before they can provide answers suitable for project decisions and licensing. There seems to be preoccupation with method development, without sufficient testing of the models against other predictive techniques and without much use of the models to develop quantitative data for project direction. Nevertheless, the PANRG has confidence that greater recognition of the importance of performance assessment as a project management tool, plus improved management of performance assessment activities by the Projects and by OCRWM Headquarters, can provide satisfactory results when needed.

CHAPTER 1

INTRODUCTION

This report documents the results of the review by the Performance Assessment National Review Group (PANRG) of the performance assessment programs and activities of three Geologic Repository Projects within the U.S. Department of Energy's Office of Civilian Radioactive Waste Management (OCRWM) Program. The PANRG was established by Roy F. Weston, Inc., (Weston), the technical support contractor of OCRWM, at the latter's request.

The highlights of this report are summarized in a separate Executive Summary and in Chapter 5. Chapter 2 contains our observations of an institutional and managerial nature. An evaluation of the technical work in the Projects is presented in Chapter 3. Reviews of a specialized nature are contained in Chapter 4.

1.1 Role of Performance Assessment in Geologic Disposal

The management and disposal of spent fuel from the operation of nuclear reactors or solidified wastes derived from the chemical reprocessing of such spent fuel, commonly described as high-level radioactive waste, is the subject of an extensive Federal program of research, development, and testing. This program is mandated by the Nuclear Waste Policy Act of 1982 (Public Law 97-425). The organization, objectives, schedules, and other features of the program are described in the Draft Mission Plan for the Civilian Radioactive Waste Management Program issued by the Department of Energy in April 1984 (USDOE, 1984a). In essence, the Nuclear Waste Policy Act and the Mission Plan call for the development of a waste management system comprised of an engineered waste package emplaced in a deep geologic repository constructed in a suitable, specially selected host rock. The system is proposed to be operational by the end of this century. It is to be licensed by the Nuclear Regulatory Commission (NRC) and must also comply with general environmental standards to be established by the Environmental Protection Agency (EPA).

The fundamental function of the waste management system is to contain and isolate the radioactive materials so they cause no undue harm to man or his environment, either now or in the future. Because this requirement extends over many millenia, it is obvious that assurance of fulfillment of the requirement cannot be demonstrated by operational experience. It can best be appraised by a systematic, quantitative evaluation using all relevant field and laboratory data combined with the most up-to-date analytical methodologies and expert scientific judgment. The term used to describe all the steps involved in predicting the potential radiologic impact of a nuclear waste disposal system, taking into account all engineered and natural components of the system, is "performance assessment."

In the United States, the regulatory performance criteria include proposed quantitative limits on cumulative releases of radionuclides to the accessible environment over 10,000 years (USEPA, 1982) and requirements on containment of radionuclides within waste packages, radionuclide release rates from the engineered barrier system, and the ground water travel time to the accessible environment (USNRC, 1981). The EPA is also considering requirements for the protection of ground water near a repository over 1,000 years (USEPA, 1984a), but the PANRG has not reviewed the Projects' approaches to demonstrating compliance with these requirements.

In general, the application of performance assessment methodologies has five major purposes:

1. evaluation and selection of repository sites;
2. guiding, and setting priorities for supporting programs of research, development, and testing;
3. development and evaluation of repository designs;
4. design and development of engineered barriers; and
5. qualification and licensing of the waste management system.

Thus, performance assessment has a vital role both in program guidance and direction, and in showing compliance with licensing requirements.

1.2 Performance Assessment National Review Group - Origin and Charter

Establishment of the Performance Assessment National Review Group (PANRG) resulted largely from the observations and conclusions of the Waste Isolations Systems Panel (WISP) of the National Research Council/National Academy of Sciences/National Academy of Engineering, which are contained in the report of the Panel entitled A Study of the Isolation System for Geologic Disposal of Radioactive Wastes (Pigford et al., 1983). The WISP concluded that the selection and licensing of sites for geologic repositories for disposal of high-level wastes will depend heavily on predicted performance of the waste isolation system. The WISP also noted that insufficient resources have been devoted to performance assessment activities. The WISP recommended a more systematic overall technical review of the program with emphasis on relating program efforts to the specific goal of developing a repository system with predictable satisfactory performance. In response to these observations and recommendations and in recognition of the importance of performance assessment as an integral part of the total program, the DOE Office of Civilian Radioactive Waste Management requested its technical support contractor, Weston, to evaluate the status of performance assessment work in the salt, basalt, and tuff projects. To accomplish this task, Weston sought the assistance of a group of outside experts - the Performance Assessment National Review Group (PANRG). The charter of PANRG is presented in Appendix A. The members of the Review Group are:

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A short professional profile of the members of the Review Group is presented in Appendix B.

The overall objectives of the PANRG as given in the charter were (1) to provide an independent review of the performance assessment work being carried out and planned by the OCRWM Projects and (2) to recommend to Weston (and through them to OCRWM) any appropriate improvements in these efforts which may be responsive to the concerns identified in the WISP report and/or which may contribute to the demonstration of compliance with licensing and regulatory requirements and the scientific and technical validity of the methodologies used.

1.3 Performance Assessment National Review Group - Procedures

The Performance Assessment National Review Group was asked to examine the work of the three projects involved in the selection and development of the first repository site. In this report, the Projects are referred to interchangeably by their initials and their rock types as follows:

Basalt	Basalt Waste Isolation Project (BWIP)
Salt	Salt Repository Project (SRP)
Tuff	Nevada Nuclear Waste Storage Investigations (NNWSI)

The review was conducted in the following way. The Review Group decided beforehand on the topics they would like to review and requested briefings on these topics by the relevant DOE Field Offices and the Projects. While the focus of the review is upon methodology, the Projects were specifically requested to present available data and results. The reason for this was that many approaches to performance assessment are well known, but in order to evaluate the quality of work by the Projects, it was necessary to examine how they are using well established techniques and the results that are being obtained. At the first meeting (April 18-20, 1984), a general orientation on performance assessment activities and plans was presented by the Projects, and staff of both the NRC and EPA described their related regulatory and standard setting activities. The EPA and NRC staff also participated in discussions regarding performance assessment activities and needs. At the second meeting held July 9-13, 1984, the Projects gave more specific technical presentations in response to an itemized request for briefings. The Group indicated that the response to our briefings request could be oral, written or both. The agenda for the two meetings and request for briefing are presented in Appendix C. The list of attendees at the meetings is presented in Appendix D.

It must be recognized that the comments in this report are based for the most part, but not entirely, on the oral presentations by the Projects and the discussions during and following these presentations. Although most presentations included hand-outs of viewgraphs used in the presentations, there were few documented results of performance assessment work provided to the PANRG. This is not necessarily a criticism, but it states the basis for this report. In some instances, the Projects provided additional materials upon request.

A draft of this report was provided to DOE-HQ, the Field Offices, the Projects, EPA and NRC for comments. The Group has considered the comments received in this final report.

CHAPTER 2

GENERAL OBSERVATIONS

This chapter contains observations of a general nature that apply mainly to managerial and institutional aspects of performance assessment. For each observation, the reasons that led us to the observation and the resultant recommendation, if any, are stated.

General Observation No. 1 - Status of Performance Assessment

Because the license application is several years in the future and few performance assessment results are available at this time, the Group sought to determine whether, in its judgment, capable staffs are available to do the job. PANRG observed that competent, professional people appear available to carry out the necessary performance assessment work. While the level of experience of individuals is variable, the adverse effects of this variability can be offset by providing contact with off-project specialists in academia and industry as well as providing for inter-project dialogue. Three kinds of experience appear to be lacking at present:

(1) experience in making reliable and defensible predictions of long-term performance of engineered and natural systems;

(2) experience in addressing specific issues related to repository performance and bringing them to closure, especially in a regulatory environment;

(3) experience in evaluating and documenting the use of professional judgments throughout the performance assessments.

Obviously, the lack of experience will be overcome as the work progresses and working relationships with the regulatory agencies develop more fully. The Review Group arrived at this observation on the basis of presentations made by the Projects and discussions with Project staffs resulting from these presentations.

General Observation No. 2 - Resources for and Use of Performance Assessment

Resources allocated to the conduct of performance assessment activities appear to be inadequate. This problem may be due to inadequate planning, the impact of difficult documentation deadlines apparently imposed by management, arbitrary priority or budgetary constraints, or perhaps to other factors. Determination of more realistic resource needs for performance assessment requires more systematic, rigorous planning and a greater emphasis on performance assessment activities.

The Review Group arrived at the above observation through the process of planning for the reviews, the degree of responsiveness of the Field Offices and the Projects to the requests for briefings, and the nature of the briefings provided. In planning for the review, PANRG encountered conflicting activities by the Projects' staffs which apparently had been judged to be of higher priority than responding to the PANRG request, be it statutory documents preparation, other meetings, or other factors. Thus, the somewhat variable quality of the briefings given to us reflects directly on the priority given to this effort by managers at various levels within OCRWM and the Projects.

The PANRG recommends that greater attention be given to the need for specific planning in the performance assessment area, i.e., the development and maintenance of Performance Assessment Plans. Obviously, such planning must be coordinated with planning in other major program areas. Of particular significance is the relation between planning for performance assessment and planning for research, development, and testing. As an integral part of the planning effort, and in view of the importance of performance assessment, careful examination should be made of resource allocation (personnel and budget) to these activities. Also included in this recommendation is increased emphasis on performance assessment studies directed toward developing better insights into program priorities within the projects. This would involve more emphasis on inclusion of uncertainty and sensitivity analyses.

General Observation No. 3 - Need for Coherent Management

The need for more coherent management in the performance assessment area was apparent. Because, as already noted, performance assessment plays a vital role in major aspects of the total program, the importance of coherent management is obvious. The apparent lack of coherence perhaps stems from the competitive approach to project management that previously existed in the program. The impact of new management and organization of OCRWM was not yet in evidence, although we understand that a Performance Assessment Coordinating Group (PACG) has been established. The organization and functions of the PACG were not presented to the PANRG. In any case, the establishment and use of appropriate management coordinating mechanisms are recommended.

General Observation No. 4 - Communications

Communication links at intra-project, inter-project, project-Headquarters, and inter-agency levels are quite evidently inadequate or inadequately utilized. A number of the participants in the two meetings of the PANRG indicated that these sessions provided one of the few opportunities to exchange ideas and experiences with fellow workers on other Projects. These meetings also provided one of the few opportunities for technical dialogue between project personnel and NRC and EPA staff. Although workshops with staff of these agencies have been held, it was apparent that their effectiveness in identifying issues and their resolution left something to be desired.

During the PANRG meetings, useful exchanges were evident among the performance assessment staffs from the various Projects. However, from informal conversations with Project personnel, an effective mechanism within the DOE-OCRWM Program for technical level exchange appeared to be lacking.

Some members of the PANRG have extensive knowledge of work in the Projects outside the framework or context of this Group. These members pointed out that the performance assessment staffs at the Projects have not taken appropriate advantage or account of hydrologic or geochemical work within their own Projects. For example, in the DOE Final Guidelines (USDOE, 1984b), favorable and potentially adverse conditions are defined which may disqualify potential repository sites. The guidelines include a list of pre-repository geochemical conditions in a host rock/ground water system that must be understood before one can judge site suitability. Favorable conditions should promote precipitation and sorption of radionuclides. Extensive geochemical work on host rock/ground water behavior of radionuclides and related species has been performed by geochemists working for the projects. Results of this work appear not to have been adequately communicated to project scientists involved in the radionuclide transport modeling effort.

Specific provisions for technical exchange on a periodic basis among project workers in the performance assessment area and also with outside specialists are recommended. Staff of the NRC should be involved in such exchanges. As part of this up-graded communication and coordination, it is also recommended that specific areas or subjects of common interest or concern to the Projects be defined (e.g., handling of uncertainty) and a coordinated effort be undertaken in these areas. Distinct, specific differences between the Projects must, however, continue to be recognized.

<u>General Observation No. 5 - Issues Resolution</u>

There appears to be an inadequate system or set of mechanisms (or they are not being adequately utilized) for identification and resolution of issues that exist or will inevitably evolve between DOE and the regulatory agencies. Examples include the difference in interpretation or definition of terms contained in the NRC and EPA regulations (10 CFR Part 60, 40 CFR Part 191) and the apparent policy of NRC not to permit use of codes by DOE in the licensing process that were developed under NRC sponsorship, purportedly because of conflict-of-interest considerations.

This observation stems from the discussions that took place following presentations by NRC and EPA staff and also reflects the experience of several members of the PANRG in dealing with the regulatory agencies and the licensing process. It should also be noted that NRC and EPA staffs indicated a willingness to discuss and engage in a continuing process of issue definition and resolution.

The PANRG strongly recommends that the Projects and OCRWM exercise more initiative in developing rational, practical interpretations of regulatory requirements and the delineation and resolution of regulatory issues. In a more general sense, this means developing a more effective working relationship with the regulatory agencies, particularly the NRC. The establishment of formal working groups to work with NRC in designated areas on a continuing basis should also be considered.

General Observation No. 6 - Scientific and Technical Basis

Based on the briefings provided, the PANRG observed that performance assessment work at the Projects appeared to be determined almost entirely by a need to demonstrate compliance with the specific regulatory requirements set by EPA and NRC. Licensing requirements do indeed provide a major focus for performance assessment; nevertheless, the need to achieve an appropriate level of understanding of the scientific and technical basis for predicting repository performance can hardly be over-emphasized. Such understanding is really the basis for the logical, defensible, and codified judgment which is the essence of performance assessment. At the same time, in a highly mission oriented program such as the development of a high-level waste repository, such understanding should be related clearly to the resolution of relevant technical issues.

While a clear distinction between what needs to be known and what would be nice to know is sometimes difficult to define, the PANRG recommends that OCRWM and the Projects develop and continuously refine a concept of "sufficient level of understanding" in order to provide a balance between the programmatic approach of meeting regulatory requirements and the desire for comprehensive scientific understanding.

General Observation No. 7 - Professional Judgment

While the PANRG regards professional judgment as a critical element in performance assessment, no formal documentation of the role of professional judgment in the Projects' performance assessment work was presented.

Professional judgment is a key element in performance assessment because it must be used in deciding, for example, which experiments to conduct, which data to use, how to interpret data, which models to choose, what are reasonable parameters for a model, what sensitivity analyses to run, how to validate codes, when an existing methodology is inadequate, and what information to communicate in reports. For many of these questions, professional judgment is not quantifiable; it is, however, essential.

In many other cases, professional judgment is used in quantifying information for analyses. Data are fit to models using judgment about which model to use and how to fit them. Probability distributions are chosen for parameters and judgment always enters into this process. In some cases, professional judgment may be all that is available about a specific situation, so general knowledge leads one to select, for example, a mean value for a probability distribution. In other cases, there may be several data points allowing one to estimate a distribution. Professional judgment is then used to decide if the data are good enough to support a reasonable calculation.

The point is simply that the basis of any performance assessment is professional judgment. It follows that if one is to build a case that a proposed repository is a good one and meets all specified requirements, then all of those professional judgments used to reach this conclusion should be documented and supported with sound logic and the best information available. This is particularly important because of the multiple scientific disciplines necessarily involved in an undertaking such as geologic disposal and because of the public scrutiny that all proposed geologic repositories and the processes to select them will receive. A significant body of professional literature in management science (Morris, 1977; Winkler, 1967), decision and risk analysis (Spetzler and von Holstein, 1975; Tversky and Kahneman, 1981), and psychology (Hogarth, 1975; Tversky and Kahneman, 1974; Wallsten and Budescu, 1983) exists on evaluating, documenting, and communicating professional judgments. Little knowledge of this work was indicated in the presentations by the Projects.

It is recommended that, in the development of a Performance Assessment Plan as noted in No. 2 above, the Projects include a discussion and clear articulation of the role of professional judgment in their performance assessment activities and how these judgments are to be identified, documented, and supported.

General Observation No. 8 - Continuing Independent Review

From PANRG meetings with the Projects and its own working meetings, the PANRG observed that a continuing, independent review of the performance assessment activities was at least highly desirable, if not essential.

Accordingly, it is recommended that such a review mechanism be established. The PANRG has no specific recommendation among the various alternatives that might be considered for this purpose.

General Observation No. 9 - Radiation Dose Calculations

Based on the form of the system performance requirements that have been developed by the EPA (USEPA, 1982, 1984a), it can be argued that performance assessment work directed towards the calculation of radiation dose or risk to individual humans is unnecessary. Nevertheless, as stated earlier, the overriding purpose of the system whose performance is to be assessed is the protection of humans and their environment from undue harm from radiation, and other parties may require or request such analyses. In particular, the Projects may, at some time, be required to show how a proposed repository matches up against developing international criteria. Probably the best developed such criteria are those recommended by the Nuclear Energy Agency of the OECD (OECD, 1984). Accordingly, PANRG concludes that the Projects should have available the models and codes that will enable them to calculate radiation doses to individuals, and that such calculations should be made. Such calculations should extend well beyond the 10,000-year period identified in the current draft EPA standard. While the presentations did not indicate that such calculational capability was being developed specifically for the Projects, there was acknowledgment by the Projects that this capability should be available. It is recommended that the capability, including the appropriate models and codes, for calculating and evaluating radiation dose to humans be available in the Projects and that such calculations and evaluations be carried out at an appropriate level. The translation of the results of such calculations to equivalent risk is also suggested. More detailed discussion and preliminary recommendations regarding environmental pathways and dosimetry modeling are presented in Chapter 4, Section 4.2.

General Observation No. 10 - Learning from Other Fields

In the course of the briefings, the PANRG observed that there are developments in other industries and disciplines which may be useful to the Projects but have not been fully utilized. For instance, in Section 3.2.4 and Section 4.4, it is observed that some techniques developed by the oil and gas industry for investigating multiphase flow in low permeability rocks may be useful to the tuff project but have not been used. These techniques are available in the published literature. In Technical Observation No. 6, it is noted that in view of the difficulties of extrapolating short-term data to geologic times, we recommend using mass transfer theory from chemical engineering (Sherwood et al., 1975). This latter approach uses only saturation concentrations of chemical species and diffusion coefficients which are measured physical parameters.

The PANRG encourages the Projects to use techniques and methods from other industries and disciplines where relevant and applicable.

CHAPTER 3

TECHNICAL EVALUATIONS

In this chapter, an evaluation of performance assessment work in the salt, basalt, and tuff projects is presented. This evaluation is obviously a "snapshot" in time, and furthermore the presentations to the PANRG could not cover details of the total performance assessment effort.

A number of technical observations are made, followed by comments related to specific performance objectives contained in the regulations. Where appropriate, the comments relate to all three Projects. A number of the comments are, however, project-specific.

Several factors tend to temper current observations relating to the technical aspects of Project performance assessment activities. These include the nature of the regulatory performance objectives and criteria, the current lack of site-specific data, competing work priorities and the general state of development of performance assessment within the Projects.

While significant reservations exist within the PANRG with respect to some of the regulatory performance objectives and criteria, which are all secondary or derived in character (protection of humans being the primary objective), the views and observations expressed below deal directly with the existing regulatory requirements, not with how the regulatory requirements might be changed. An important aspect of the licensing process is the fact that only one repository system will be put into operation in this century and, most likely, only two such facilities will be operated through the first half of the 21st century by a single licensee. Thus, repository licensing represents a decidedly different situation than that associated with the licensing of nuclear power reactors, where regulatory interpretations for one licensing case become precedents for many other licensing cases.

While the Projects have much in common (e.g., uncertainty and sensitivity analytical methods, dose calculations, far-field hydrologic transport models, leaching data and correlations), the Projects are distinctly different because of their different hydrogeologic settings. This difference quite naturally leads to some differences in performance assessment models, the inputs to those models, and perhaps even to some differences in performance assessment approach, as well as to differences in interpretation of regulatory performance objectives and criteria.

3.1 Technical Observations

<u>Technical Observation No. 1 - Definitions and Interpretations</u>

An obvious need exists for clear and mutually-agreed-to definitions and/or interpretation of terms contained in the NRC and EPA regulations or used in connection with these regulations. Where feasible, uniform definitions should be sought. In some cases they may well differ between the Projects, but the definitions/interpretations must be agreed to by the individual projects and the regulatory agency. Existing technical terms should, of course, be defined in conformity with accepted scientific usage. Among the terms which appear to require more uniform understanding are:

- Significantly disturbed zone
- Engineered barrier system boundary
- Radionuclide release rate from engineered barriers system
- Terms related to ground-water movement, (viz, travel time, fastest path)
- Accessible environment
- Substantially complete containment
- Realistically conservative vs. best estimate
- Preliminary performance assessment
- Scenario - is it a projected single event or process, a sequence of events/processes as they exist at a point in time, etc.
- Reasonable expectation
- Reasonable assurance

Other regulatory requirements or definitions whose ambiguity would cause difficulty in performance assessment should also be dealt with.

It is recommended that a coordinated effort involving OCRWM and the Projects be undertaken to develop appropriate definitions and interpretations of specific regulatory requirements and language. These should be presented to the regulatory agencies for review, discussion, and formal concurrence. While uniform definitions are sometimes possible, some concepts and terms have site-specific meanings or implications, and these should be accommodated.

Technical Observation No. 2 - Team Approach

The development of models for use in performance assessment is basically a codification of technical judgment. Such codification appeared to be primarily the work of the performance assessment staff rather than more of a joint effort of those working in performance assessment, including laboratory and field engineers and scientists. The need for such joint efforts (including cooperation among the Projects) is important now and likely will become increasingly important as the planning and conduct of in-situ testing proceeds.

The PANRG recommends that more of a team or task force approach be used in the development of performance assessment models. Those involved in predicting performance and laboratory and field staff should comprise the team. It is expected that this would foster the development of a sound scientific basis for the modeling effort and also ensure that the field and laboratory research programs are focused on developing the information essential to performance assessment. The strategy should be based on the identification and modeling of the key phenomena that control radiation dose to humans which is one of the basic objectives of waste isolation.

Technical Observation No. 3 - Predictive Reliability and The Use of Bounding Analyses

Predictive reliability, i.e., the assurance that the actual performance will be as good or better than that stated by the performance prediction, is important for any engineering project. Predictive reliability is essential for a geologic repository because real-time testing to confirm the repository design and to confirm the predictions of long-term performance is impossible. The expected long-term performance of repositories should also be predicted. As is discussed below, in any system design the use of well established and easily verified calculational techniques to establish the bounding values of predicted performance should be balanced with the desire to refine the performance prediction for greater realism.

Bounding analyses can be used to establish predictive reliability and to estimate limiting features of system behavior. In some instances, physically unrealistic assumptions or input values are used to obtain a conservative "bounding" result. For example, when calculating the cumulative release of radionuclides, the assumption that all the ground water flowing through the repository becomes saturated with respect to the radioelements in the waste or with respect to the waste-form UO_2 matrix is unrealistic. However, if the values chosen for the saturation concentrations and water flow rates are defensible, then the calculated release is defensible as a conservative bound and the result is expected to be reliable. If the predicted releases are suitably below the release limits established for acceptable performance, then the bounding calculation may be sufficient to demonstrate that the repository will more than meet the regulatory criteria. In presenting such results, however, the nature of the conservatism should be specified. Furthermore, the fact that the actual performance is likely to be far better than represented by the bounding calculations should be stated clearly. A word of caution, also, should be added to the effect that future changes in the available data should not be used to revise release figures without undertaking a thorough reevaluation of the entire bounding calculation.

Wherever possible, performance analysis should proceed beyond simple bounding calculations to obtain more realistic estimates of expected performance. For example, because the emplaced waste packages are discrete and separated from each other, it is impossible for all water potentially flowing through a repository to become saturated with any waste constituent, assuming it is not already saturated with that constituent before encountering the waste and assuming no large changes in saturation concentration in the repository environment. The only place that concentrations near saturation are expected is in the liquid immediately adjacent to the waste surface. All other water will be below the saturation concentration, and the average concentration in ground water leaving the repository will be below saturation.

The average concentration of a species dissolved from the waste can be estimated by a more realistic calculation, such as that used in mass-transfer analysis. However, if this more realistic calculation is obtained by assuming that all of the waste solid is suddenly exposed to ground water for dissolution and diffusive-convective release when the corrosion-resistant barrier fails it is still bounding, though more realistic and less conservative than the first calculation described.

If the simpler and more conservative bounding calculation shows compliance with well established limits and if it requires the least amount of data, then it is the most easily validated and can be expected to result in reliable predictions, however unrealistic and conservative. As the complexity increases, however, more phenomena, assumptions, and input data must be validated, and predictive reliability is more difficult to obtain.

Further realism is usually expected to result in lower predicted releases. For example, not all of the protective container is expected to fail at once, and releases from the waste solid will likely be reduced by the tortuous pathways through the partially failed outer layers and corrosion products. The multicomponent corrosion products can result in solid phases that reduce the saturation concentration of the dissolving species. As we recommend later, the protective features of these more realistic phenomena should be taken into account in performance assessment, where possible. However, in any predictive effort there must be a compromise between the increased detail for realism as contrasted with the loss of predictive reliability when the increased detail requires more data and validation than is possible with available resources and time. This kind of compromise arises in all facets of the prediction of repository performance.

The PANRG recommends that every phase of repository design, development, and performance prediction be carefully evaluated to achieve a proper balance between bounding calculations and realism, focusing on predictive reliability as a necessary result. A related recommendation from the PANRG is in three parts. First, where the application of science and technology has provided reasonable values, they should be used for analytical purposes. Second, while bounding analyses are useful in demonstration of regulatory compliance, the results of such analyses are less useful in comparing different repository sites or different repository designs. Third, when results of bounding analyses are displayed in terms of consequences, the associated probability of exceeding those consequences should also be shown.

Technical Observation No. 4 - Extrapolation

Little or no explanation or description was given of the bases for extrapolating current or historical data obtained in the laboratory or field (e.g., corrosion and dissolution data, geologic properties that control ground-water travel times) to the long periods involved in geologic isolation. In the case of waste form dissolution rates, there was some awareness indicated of the existence of related data from other countries (e.g., Johnson and Crosthwaite, 1984; SKBF/KBS, 1983), but there did not appear to be, as yet, any significant effort to compare or correlate these data on predicted long-term dissolution rates. The need for technically defensible bases for such extrapolation was acknowledged. However, the special concern expressed in the WISP report about the problem in extrapolating real-time rate data on dissolution rates and corrosion evidently has yet to be addressed.

Some Project staff argued that the empirical rate laws developed over periods of months to a few years could be extrapolated in time and with temperature for application to the postclosure period. However, initial rate laws often depend on the concentrations of reactants, whereas later in time, near saturation with the solid phase being dissolved, the rate law changes form and may well depend instead on the degree of saturation of the ground water with respect to the phase. On the same point of extrapolating in time, little or no discussion was presented of the usefulness of information on the natural water/rock system, or on analogue systems such as contact metamorphic or hydrothermal systems, to assist in the prediction of the long-term behavior of a repository. These approaches may provide a unique and otherwise unavailable means of predicting such behavior. For example, studies of natural water/rock systems have shown that leaching rates of uraniferous rocks under natural conditions are generally much slower than measured in the laboratory, frequently by two or more orders of magnitude (Pigford et al., 1983).

Long-term climatic fluctuations and associated phenomena could result in major changes in the hydrogeologic system such that predictions (e.g., water transport velocities) based on short-term observations of geologic processes could be vastly different than those which would actually occur in the future. The range of possible future fluctuations can be estimated most accurately by studying geologic and geochemical evidence of past fluctuations on a site-specific basis. Also, the geochemistry of the ground-water system is clearly a critical factor in determining radionuclide retardation relative to ground-water movement. Consequently, rational predictions of long-term transport of radionuclides cannot be accomplished without data based on geologic and geochemical reconstructions.

One approach for handling this difficult problem is to obtain as much information as possible concerning the natural fluctuations in the past hydrogeologic systems which will serve as a constraint to projections of possible ground-water transport phenomena in the future. In short, the past is the best key to the future. The past can be understood in part by geomorphic reconstructions of various factors related to climate. Most important, and not discussed by those giving presentations, however, is the use of general geochemical and isotopic data derived from studies of ground water and of late Pleistocene deposits of secondary minerals. Such studies will constitute the only direct validation of otherwise tenuous long-term hydrogeologic projections.

The PANRG recommends that more fully developed and technically defensible bases be pursued for extrapolating results of short-term laboratory and field investigations to the long times required in performance assessment. This should include the kind of geochemical investigations and analyses indicated above.

<u>Technical Observation No. 5 - Spent Fuel Characteristics</u>

Spent nuclear fuel will be the major waste form from civilian power reactors to be placed in the first repository. While we now have extensive data on the dissolution rates of borosilicate glass in the laboratory environment (Mendel, 1984), and of more recently developed waste forms (Oversby, 1982; Sales and Boatner, 1984), the equivalent data base for spent fuel in reducing redox environments does not exist. A considerable amount of information does exist on Canadian CANDU fuel (Johnson & Crosthwaite, 1984) although it is important to recognize that there are significant differences from US fuel in fuel design and burnup.

Based on the conclusions presented by the tuff project, the Zircaloy fuel cladding is of potential significance as a component of the waste package because:

- it contains about half of the total carbon-14 in the waste package, and this portion would be released when the cladding corrodes;
- if the cladding corrodes slowly enough (over time periods greater than 10,000 years as stated by LLNL for the tuff project), and if it is not penetrated by stress-induced failures and by other mechanisms, then the cladding obviously assures compliance with the 300-1000 year NRC containment requirement for those radionuclides within the UO_2 matrix;
- if cladding failure is by local cracking or penetration and such failures are statistically distributed over long periods of time (e.g., thousands of years), then the effective release rate of radionuclides from the waste form could be much lower than if all the UO_2 is assumed to be exposed to groundwater at the same time.

Although the technical bases for these conclusions were not presented, if the NNWSI/LLNL estimates are correct, then the Zircaloy cladding could be a significant barrier for radionuclide transport in the basalt and salt projects as well, depending upon its corrosion rate in the different environments. Obviously, a comprehensive review of Zircaloy corrosion data is indicated.

Some spent fuel leaching data are known to be available from foreign programs but up-to-date knowledge of these data was not reflected in the presentations to the Group. Calculations made by the Projects to estimate release rates from spent fuel rely upon bounding calculations based on volumetric liquid flow rates and solubilities, or they are based on mass-transfer analysis that assumes saturation at the inner surface of the backfill; none have relied upon laboratory leaching data. PNL is to provide SRP/ONWI with some predictive correlations of spent-fuel leaching data to use in estimating release rates with water intrusion.

The tuff project plans to obtain its own data on radionuclide release from spent fuel in laboratory tests of components of fuel, cladding, and rock. Even without such data, NNWSI concludes that the release rates of all radionuclides from spent fuel will meet regulatory requirements, based on the latest estimate of the water infiltration rate at the repository horizon, uranium solubility, and the assumption of congruent dissolution of all radionuclides other than those (especially cesium and iodine) in the fuel grain boundaries, in the fuel-cladding gap and gas plenum, and in the Zircaloy cladding. They conclude that the release rate of all such radionuclides not in the fuel matrix will be at a rate less than the regulatory criteria because of long-term statistical failures and failure rates of the cladding and canister. These assumptions need be justified, tested, and quantified.

The fuel-release calculations by BWIP and SRP indicate that these projects may need data for the release rate of more soluble radioelements, e.g., Cs, I, C, and others, from spent fuel to determine if these release rates are slow enough to aid in compliance with NRC's regulation. These data are also likely to be important for the NNWSI project.

The PANRG recommendations related to these observations are explicit, namely:

a) a comprehensive review of Zircaloy corrosion data should be conducted; with emphasis upon extent of hydriding embrittlement and cracking of Zircaloy cladding in discharged fuel, additional hydriding and cracking in the repository enviroment, failure mechanisms, and quantitative characterization of statistical failures (effective sizes, number, and distribution with time of cladding penetration in the repository environment; leach rates of carbon-14 and effective solubilities of released carbon).

b) a similar comprehensive review of corrosion and failure data for canisters and overpacks; and

c) an adequate data base on the dissolution of radionuclides from spent fuel and from the fuel matrix should be developed, with special emphasis on developing data on leach rates for the more soluble radionuclides and apparent solubilities for all of the radioelements.

Technical Observation No. 6 - Mass Transfer Analysis

In view of the last two Technical Observations regarding the lack of data on spent fuel and the difficulty of extrapolating leaching data for long periods of time, the PANRG observes that there may be alternative methods for calculating the source term and recommends that these methods be considered. The Projects are urged to make more extensive use of mass transfer analysis (Sherwood et al., 1975), which is the detailed and quantitative investigation of mechanisms, processes, and rates for the transfer of materials between phases. For example, Chambre' and Pigford (1984) have developed techniques that predict the rate of transport of dissolved species from the waste-package surface by molecular diffusion and convection in ground water in backfill and in the surrounding rock. The simplest form of their theory requires only the measured values of saturation concentration of radioelements and diffusion coefficients in the groundwater; no leaching data are required and assumptions and uncertainties in the long-term extrapolation of leaching data are avoided. The theory requires no arbitrary or adjustable parameters to predict dissolution rate. A similar approach to predict the corrosion lifetime of the fuel canister has been used in Sweden (SKBF/KBS, 1983), and mass-transfer analysis has recently been introduced at the BWIP project.

The predictive techniques of mass transfer and of near-field and far-field radionuclide transport can now estimate release rates and releases at various distances from a waste form. Furthermore, development of this work may provide an approach for performance analysis and for demonstrating compliance with regulatory requirements that is more credible and reliable than can be obtained from uncertain extrapolations of data from laboratory leach tests and from similar experiments.

The mass transfer approach was endorsed by the WISP panel. The PANRG recommends that the Projects consider making greater use of these techniques.

Technical Observation No. 7 - Verification and Validation

Verification and validation of models used in performance assessment clearly will be a key issue in the eventual licensing of geologic repositories. The PANRG specifically requested that it be informed of validation efforts associated with each model described to it, but related presentations were necessarily incomplete. PANRG observed several fundamental difficulties in this regard.

First, the requirements for verification, benchmarking, and validation were not defined clearly. Definitions that are acceptable to OCRWM and NRC are needed, otherwise the basis for performance assessment results may be unnecessarily open to question, or unnecessary effort might be expended on the verification/validation process. An operational definition is particularly important in the case of model validation. Because of the long time periods over which repository performance must be predicted, most performance assessment models cannot be validated directly and completely (i.e., direct comparisons of model predictions with actual repository performance cannot be obtained).

The validation of far-field hydrologic models which are used for long-term projections of the possible transport of anthropogenic radionuclides is a particularly troublesome task. Vital information concerning past hydrologic conditions averaged over long periods of time is, nevertheless, commonly available from the water itself. Subsurface residence times for water can be estimated by measuring: (1) the decay of atmospherically derived radionuclides (hydrogen-3, carbon-14, chlorine-36, argon-39, and possibly krypton-81); (2) the subsurface build-up of radiogenic gases (helium-4 and argon-40); (3) the degree of radioactive disequilibrium (uranium-234/ uranium-238); (4) the variations of chlorine, oxygen-18/oxygen-16, hydrogen-2/ hydrogen-1, argon, neon, xenon and krypton, and other climate-related constituents which in turn will allow correlations with known climatic fluctuations; (5) the time-related changes in ions and molecules (oxygen-18 isotopic disequilibrium in sulfate water and amino acids); (6) the presence of anthropogenic constituents (tritium, chlorine-36, krypton-85, and the Freons); and (7) various constituents which can be related to datable geologic events, such as chloride from a former high-stand of the sea. Although gas movement through the unsaturated zone may preclude the use of noble gases for many purposes at Yucca Mountain, other elements such as carbon and chlorine can yield useful information on the movement of water in the subsurface within the unsaturated zone.

In using geochemical information involving natural isotopes, it is important to recognize that water samples from the subsurface are always mixtures of waters from various sources. The sources of these waters may be quite divergent in origin or they can be almost, but not quite, identical. The mixing takes place as a natural dispersive process within aquifers as well as within the drill holes used for sampling. The way in which this mixing affects the usefulness of geochemical studies is commonly misinterpreted. Rather than negating geochemical studies, as some would claim, the presence of mixing is one of the strongest arguments for the urgent need of geochemical studies, because they represent about the only direct method of studying mixing phenomena in large-scale natural systems. Another common misconception is that only one or two isotopic methods will by some magic produce abundant information on mixing, flow directions, and residence times. While in some natural systems this might be true, most commonly a large number of constituents should be studied in order to extract an optimum amount of information. It should be remembered that each constituent dissolved in the water is there because of a unique sequence of events in the history of the water. Taken individually, these constituents reveal small segments of the history of the water; taken collectively, they yield information essential to performance assessment.

Second, the PANRG observed that various codes being used by the Projects are in different states of verification and validation as defined by the Projects. For example, some far-field, regional ground-water flow models have been validated for some applications (Pearson et al., 1983). Others have been benchmarked and verified as defined by the basalt project (Arnett et al., 1984; Eyler and Budden, 1984).

In addition to setting up the process for verification and validation, it is important that there be effective mechanisms for evaluating and confirming the results of the verification/validation process. A process itself does not necessarily achieve the desired results. For sample, a waste package performance code called WAPPA (INTERA, 1983c) has been identified by each of the Projects as one of the codes that they will use for waste package scale performance assessment (ONWI, 1984; Rockwell Hanford Operations, 1984). No reservations were expressed concerning the adequacy of the WAPPA code to carry out what is claimed, including its predictions of rates that radionuclides are released from a waste package. However, in reviewing parts of the WAPPA code, it was found that it calculates the time-dependent diffusion of radionuclides through backfill using a finite-difference formulation based on an analytical solution for steady-state diffusion with no convective transport. Even without convective transport, errors introduced by the steady-state approximation can easily be evaluated, but evidently this has not been done. The manual states, without justification, that steady state diffusive transport will occur within several decades, a result that is in conflict with results from other calculations in the DOE program. The mass-transfer results calculated by WAPPA are not necessarily conservative. The manual speaks of an "adjusted diffusion coefficient" for these calculations, but it does not describe how the coefficient is to be adjusted or obtained. Some terms in the equations are introduced without definitions adequate for independent checking. The same steady-diffusion equations are assumed to apply also when there is finite flow of ground water in the backfill, and the combined diffusive-advective transport through the packing is calculated by assuming that the contents within the backfill are at all times well mixed. No test of the validity of this assumption is presented.

The only verification described in this part of the WAPPA manual is a hand calculation to see if the finite-difference equations described in the manual give the same numerical answer as a computer run for zero flow. The limited range of parameters considered may not be an adequate check of computer arithmetic. The validity of the formulation itself could be checked, but there is no record that this has been done. The code assumes, without discussion or justification, that diffusional transport through holes of known area in the canister is given by the diffusional transport for a completely failed canister corrected by the ratio of total hole area to canister area. This assumption is not in accord with diffusion theory and is not conservative. WAPPA's assumption of zero concentration of radionuclides in ground water outside the backfill simplifies the source-term calculation and leads to a conservative but unnecessarily high estimate of the rate of mass transfer through the backfill. More accurate and realistic calculations of mass transfer through backfill are already carried out by other techniques at BWIP and elsewhere and are available to the other Projects. The fact that all the Projects list WAPPA as one of their key codes, with no reservations about its validity, indicates that the verification/validation process is not always effective. Quality assurance of prediction is as important as quality assurance of construction. Reliable techniques that implement that necessary evaluation need to be instituted.

Another example of the need for careful evaluation of results, as part of the verification/validation process, arises from BWIP's calculation of mass-transfer from a waste package and backfill using the stochastic version of the finite-element code CHAINT (Baca et al., 1984). BWIP presented release rates for selenium-79, of 65,000 year half life, from bentonite backfill 0.15 m thick and 1.5 m thick. The results showed that the thicker backfill resulted in lower release rates during a 10,000-year time interval. BWIP quoted a backfill porosity of 20 percent and an effective porosity of surrounding rock of a few percent. For such conditions, other studies, e.g., Chambre' et al. (1983), have shown that removing more rock to allow for thicker backfill results in greater release rates for long-lived radionuclides, because the backfill porosity is much greater than that of the rock that it replaces. Evidently the contradictory results by BWIP stem from their use of a zero-concentration boundary condition at the outer surface of the backfill, thereby neglecting the important diffusive resistance in the surrounding rock. Also, it was pointed out that in these calculations BWIP adopted a molecular diffusion coefficient characteristic of compressed bentonite, with greater tortuosity than is expected for the relatively loose backfill.

The code CHAINT may well be formulated correctly and it may give precise and correct results for the problem that is asked to calculate. However, a code can be used to give incorrect results, results that can lead to incorrect conclusions. This illustrates that an essential part of verification/validation is the evaluation of the results that are obtained.

The publication supplied to the Group in support of the CHAINT mass transfer calculation did not contain the essential parameters and boundary-condition assumptions necessary to make an independent judgement of the adequacy of the calculation. These were obtained through further discussion with BWIP representatives. More complete documentation can aid peer review and contributes to verification/validation.

BWIP has the capability of both analytical and finite-element mass-transfer calculation of radionuclide release rate. Comparing the results from these two approaches, as well as comparing with results from the mass-transfer portion of WAPPA and other published work, would aid in the verification/validation of these models.

OCRWM should undertake with NRC the development of mutually agreeable requirements for verification and validation, and that the OCRWM assign a high priority to the verification and validation process consistent with those requirements.

<u>Technical Observation No. 8 - Uncertainty and Stochastic Analyses</u>

Uncertainty about the eventual performance of a repository is a major issue in licensing. Various interest groups are also keenly concerned about the uncertainties related to the long-term safety of high-level waste disposal. The techniques and methodologies available and under development for uncertainty analysis in the Projects appear to be adequate. However, based on the Projects' presentations, the potential usefulness of uncertainty analysis at this stage in performance predictions is not being fully realized. Furthermore, the incorporation of uncertainty analysis into various computer codes was still mostly in the planning stage.

The Projects should draw a clear distinction between spatial or temporal <u>variability</u> as opposed to the <u>uncertainty</u> of parameters. For example, natural aquifers display spatial variability in hydraulic conductivity (see Figure 4.6). This variability can be characterized by the statistical properties of the spatial distribution, such as the mean, variance and spatial correlation length. Uncertainty refers to, for example, the lack of knowledge about the variation in the input data and in the accuracy of the models used. Sources of uncertainty include measurement error, lack of understanding of the physical processes of the system, and extrapolation into the distant future. In addition to uncertainty and variability, certain phenomena in nature are best considered as random and are most appropriately characterized by a probability of occurrence.

There are several approaches to handling uncertainty and variability. One approach is to build stochastic considerations directly into the models. For instance, the stochastic hydrology methods discussed in Section 4.1 incorporate the statistical properties of aquifer variability in the determination of tracer distributions in space and time. Uncertainties in aquifer parameters can be examined by undertaking sensitivity studies, for example, through varying the statistical properties of the parameters.

The more traditional method of dealing with uncertainty is to formulate the governing equations in a deterministic manner and represent variables such as hydraulic conductivity by a single estimate. Probabilistic results due to uncertainties in input parameters can be explored by methods such as random sampling (Monte Carlo). If such an approach is used, then a probability distribution has to be specified for the input parameter or parameters. In the case of hydraulic conductivity, a lognormal distribution is often assumed. It should be pointed out that the lognormal distribution for hydraulic parameters is unproved for extreme values. The use of such parameters obtained by extrapolation of a lognormal distribution should be justified specifically rather than being accepted as giving "conservative" (but possibly unrealistic or erroneous) results. On the other hand, it is not correct to assume a uniform probability distribution for a parameter because there is "no information," as claimed in one project presentation (Drake, 1967).

An example of the need for a stochastic approach is meeting the "fastest water travel time" requirement of the NRC regulations. Aside from the need for a mutually understood interpretation of the term, the use of a single discrete value for this factor could lead to unnecessary difficulty. It would seem much more reasonable to characterize this factor in the form of a probability distribution. Providing assurance of an even longer mean water travel time than that currently required by the existing regulations would seem reasonable with such an approach. For example, the regulation might require the mean travel time to be greater than 1200 years.

It is recommended by the PANRG that greater emphasis be placed on uncertainty analyses, since significant insights can be derived from such analyses. Coordinated with reasonable sensitivity analyses, these insights can also help set project priorities and assist in project decision-making. The PANRG also recommends that the Projects use stochastic approaches in their performance assessment where appropriate and applicable.

Technical Observation No. 9 - Sensitivity Analysis

Many of the performance assessment models presented to the PANRG are highly complex and contain large numbers of variables. Sensitivity analyses would provide quantitative estimates of the relative importance of these variables. The PANRG found some of the techniques being considered for sensitivity analysis, such as the adjoint method, extremely interesting and powerful. The PANRG would have liked to see some actual application of such techniques on performance assessment models.

The PANRG noted two aspects of the Projects' sensitivity analysis work. First, there is indication of uneven development of techniques and methodologies among the Projects. Second, there was little indication of the effective use of sensitivity analysis results in project management, such as setting priorities in data acquisition.

Accordingly, the PANRG recommends improved inter-project coordination on approaches and methods for sensitivity analysis and more extensive use of results of sensitivity analyses to set priorities for data acquisition.

Technical Observation No. 10 - Hierarchy of Models

A broad variety of models has been developed by the Projects to represent the various components of the repository system, the physical and geochemical processes acting on these components over time, and the processes involved in flow and transport of radionuclides. The approach of having a hierarchy of models ranging from simple to complex that are consistent with the characteristics of the pertinent data base appeared satisfactory, especially as done in the tuff project. However, in the presentations the Projects did not fully describe the capabilities of their systems models to the Group.

In contrast, the role of different types and levels of models is clearly stated in the Canadian performance assessment program. The Canadians use "research" or very detailed models to investigate natural phenomena, such as three-dimensional numerical codes for ground-water flow modeling, and then use their systems model SYVAC (Lyon, 1981) for uncertainty and sensitivity analysis.

The PANRG recommends that each of the Projects develop a full description of the hierarchy of models and overall systems model that they plan to use in performance assessment. This description, which should delineate the relationship between the different types of models, would be useful in informing interested parties on the scope and nature of the Projects' performance assessment activities and in comparative evaluations of repository sites.

Technical Observation No. 11 - Use of Geochemical Data

Throughout the review process, the PANRG observed inadequate utilization of geochemical information in performance assessment. Such information and geochemical models can provide useful insights in corroborating the results of performance assessment. For example, Hubbard et al. (1983) and Hubbard and Laul (1984) have analyzed deep brines from the Palo Duro Basin of north Texas for their activities of natural uranium-238 and thorium-232 and their daughter products. They found equal activities of radium-226 and of its daughter radon-222. Radon-222 is a gas and not adsorbed, indicating that radium-226 is also not adsorbed. Equal brine activities of radium-228 and radium-224 (the daughter of intermediate thorium-228) gave further evidence that radium is not adsorbed. These are examples of results of geochemical studies which can guide the prediction of the fate of radionuclides, such as radium-226, should they be released from a breached repository.

The PANRG's observation is that geochemical tools do not appear to be an integral part of performance assessment in the Projects. The PANRG also noted that site-specific geochemical data are not yet fully available since they will be obtained in the site characterization process.

In addition to obtaining an internally consistent single set of thermodynamic data for important radioelements, the PANRG recommends that priority be given to obtaining geochemical data during site characterization, with emphasis on background water chemistry as well as solubilities and adsorption behavior of relevant radionuclides and related species.

Technical Observation No. 12 - Coupled Processes

The commonly identified coupled processes are chemical-thermal-hydrologic-mechanical, and, in the repository environment, radiological effects (Tsang and Mangold, 1984). Consideration of these coupled processes is important for performance assessment because most aspects of repository performance will be the result of interactions among the basic processes. For instance, as the rock surrounding the repository is heated, under certain circumstances one could expect precipitation of $CaCO_3$ and $CaSO_4$, accompanied by the dissolution of silicate minerals near the waste packages and precipitation of silica in pore spaces some distance away at lower temperatures. Another effect might be radiolysis-induced chlorine formation, enhanced by temperature, causing canister corrosion. The Projects currently use a number of models to describe and predict ground-water flow and transport. Some of these consider coupling of hydrological-thermal and simple chemical processes. The PANRG recommends that as a priority item, the Projects consider the importance of coupled processes in performance assessment.

Technical Observation No. 13 - The Role of Dispersion

The Projects provided general discussion of methodologies for predicting hydrogeological transport of radionuclides, including stochastic techniques for predicting dispersion effects and including the use of site-dependent dispersion coefficients. Few results from the application of these methodologies were described. Plans to acquire data on dispersion coefficients were not yet well developed, and it was recognized that obtaining appropriate site-specific data may be difficult, particularly for the tuff project which utilizes a complicated flow and transport calculation that distinguishes between dispersion coefficients for the porous rock matrix and dispersion coefficients for fractures.

If accurate predictions of dispersive transport are needed for predicting long-term performance, then an extensive field test program must be planned and initiated for each of the projects. However, the importance of dispersive transport in performance predictions was not clearly established. It was thought by the Projects that dispersive effects would have little effect upon the predictions of 10,000-year cumulative release at the accessible environment, but no quantitative results were presented to support this conclusion. Cumulative release is likely to be insensitive to dispersion unless EPA's proposed 10,000-year cutoff is taken literally and if the predicted time for radionuclides to reach the accessible environment by advective transport is approximately 10,000 years. This can occur for some radionuclides and should be examined now by the projects. Rather than undertake an extensive program to develop dispersion data for precise predictions of environmental release before an arbitrary 10,000-year cutoff, it would be prudent to extend the time period of the calculations so that early transport by dispersion is not important to the estimated cumulative release.

The projects have evidently not examined the possible effects of dispersion on meeting the NRC's release-rate criterion, although it is evident that the simple bounding calculation of release rate adopted by the salt project will not be affected by hydrodynamic dispersion. The mass-transfer calculation of release rate adopted by the basalt project will not be affected by hydrodynamic dispersion because the local mass transfer from the waste package is expected to be controlled by molecular diffusion. However, if the Projects conclude that the release-rate criterion is to be met at greater distances from the waste packages, such as at the ceiling of a backfilled drift with floor-emplaced waste, or beyond, then the issues of hydrodynamic dispersion could become important in predicting local release rates. Also, these distances may be such that stochastic methods are needed for accurate predictions of radionuclide transport at greater distances. However, to meet the NRC criterion, it is the fractional release rate integrated over the outer surface of the engineered barriers that is important. For a long-lived species with no precursors, continuity will require that the temporal total release rates across the engineered barrier surface, once the species has reached the surface, will be near, but not greater than, the temporal total release rate of that species from the waste package. Therefore, after the radionuclide species have reached the engineered barrier surface, the integrated fractional release rate may be relatively easy to predict, and the maximum value of the integrated fractional release rate may be insensitive to dispersion. The projects should conduct such studies to determine whether dispersive effects on maximum fractional release rates at various distances are important for the important radionuclides.

Hydrodynamic dispersion will broaden the concentration bands of radionuclides undergoing hydrogeologic transport, and it can considerably reduce the maximum far-field concentrations of radionuclides if the time span of radionuclide release is short enough or if the time of radionuclide transport is long enough. Dispersion can thus affect the predicted repository performance if the performance criterion relates to maximum temporal concentration in ground water at some distance well removed from the emplaced waste (i.e., if an individual radiation dose criterion is applied). However, even for an individual dose criterion, dispersion effects are not always important, depending upon the time span of release from the waste package and the time of radionuclide transport. The Projects should conduct prediction studies to identify for which radionuclides dispersion is important in affecting far-field concentration. Also, they should estimate what precision of dispersion data are needed to make suitable performance estimates of maximum individual doses.

In discussions of how to interpret and comply with NRC's criterion for ground-water travel time, it was suggested that an extreme interpretation could require dispersion calculations to estimate the time for fastest-moving ground-water parcels to travel along the shortest path length. In examining the stated purpose of the water-travel-time criterion, we find no justification for such an extreme interpretation. An extensive program of dispersion analysis and measurement should not be justified on such grounds.

It is timely that the role and importance of dispersion in repository performance predictions be better analyzed and understood by the projects before extensive effort is committed to stochastic analyses and field tests to obtain site-specific data on dispersion.

3.2 Evaluations

Table 3.1 is a summary evaluation by the PANRG of the performance assessment work in the basalt, salt, and tuff projects. Detailed comments with respect to each regulatory performance requirement follow.

3.2.1 Containment Requirement

Section 60.113(a)(1)(ii)(A) of the NRC regulations calls for "substantially complete" containment of radionuclides within the waste packages for 300 to 1000 years. In the salt and tuff projects, the waste package will consist of the encapsulated waste form plus a metallic container called a canister. In the basalt project, there is proposed a layer of bentonite and crushed basalt surrounding the outside of the metal canister. The corrosion of the metal canister and containment or transport of radionuclides through the packing material proposed by the basalt project is discussed below.

Different metals are used as canisters by each of the Projects due to the different chemical environments. Each project is carrying out corrosion tests in liquids simulating the repository environments. The Projects presented predictions of containment life that (1) assumed that corrosion rates are spatially uniform over the entire surface of the metal container and (2) assumed that corrosion rates will remain constant for several hundred years at the rates established in laboratory tests of duration from months to a few years. Information presented to the Group did not provide adequate justification for these two important assumptions.

The chemical mechanisms and rate laws that control long-term corrosion and failure of these metals in repository environments are not known. It does not appear possible now to interpret long-term corrosion from accelerated corrosion experiments. We recommend peer review by a selected group of experts, including those knowledgeable about the geochemical environment, failure mechanisms of fuel cladding, fundamentals of metal corrosion and the design of components and structures for long-term containment integrity, to evaluate the predictive reliability from the approaches now taken by the Projects.

The WISP report recommended special attention to corrosion during the transient environment following waste emplacement and sealing, including water-line corrosion. This has been addressed only to a limited extent. The Projects and NRC are studying various other forms of corrosion, such as pitting, crevice, stress-corrosion cracking, and hydrogen embrittlement. The phenomena must be understood and quantified before reliable predictions of corrosion life and failure rates can be made.

The WISP report also pointed out that complete containment of all waste packages for a specified period is likely to be impossible because of expected manufacturing imperfections. If the NRC interprets its 300-to-1000-year containment criterion as applying only to a significant number of the waste packages, which is an expected and reasonable interpretation, then the impact of containment failures distributed statistically over time should be considered. This could decrease the instantaneous release rate of

TABLE 3.1 Summary of PANRG Evaluations

	REQUIREMENTS					
	CONTAINMENT IN WASTE PACKAGE	RELEASE RATES	TRAVEL TIME	CUMULATIVE RELEASE	DOSES	UNCERTAINTY ANALYSIS
AUTH-ORITY	10 CFR 60.113(a)(1)(ii)(A)	10 CFR 60.113(a)(1)(ii)(B)	10 CFR 60.113(a)(2)	41 CFR 191		
ALL	Assuming only uniform corrosion a probable licensing issue. Need defensible basis for extrapolation to geologic time scale. See Section 3.2.1 and Technical Obs. 4 & 5	Need to obtain site-specific solubilities of chemical species of relevant radioelements. See Section 3.2.2 and Technical Obs. 4 & 6	Need definition of compliance with this requirement. Need to emphasize that it is mass flux that will transport radioactive elements, pore velocity may not be significant. See Section 3.2.3 and Technical Observation 2	Need to identify the nature of release scenarios and their associated probabilities. See Section 3.2.4 and Technical Observation 7	Not Reviewed See Gen. Obs. 9	Should consider sharing approaches and methodologies. See Technical Observations 8 & 9
SALT	Assuming only uniform corrosion and extrapolating to geologic time scale, probable licensing issue.	Good bounding calculations based on physical nature of salt, and several postulated mechanisms of transport. Need site-specific data and a defensible theory for brine migration.	Current estimate of brine diffusion coefficient from a single observation may be questioned in licensing.	Assumes complete containment of radionuclides. Bounding analyses indicate within EPA limits. Need to consider modeling of seals and plugs.		Combination of adjoint and random sampling potentially powerful technique. Need to see practical application to performance assessments.
BASALT	Presentation to PANRG included only a model for uniform corrosion of canister/overpack. Based on this information, the Group considers the approach probably inadequate for licensing.	Bounding calculations initiated. Presentation to PANRG included a one-dimensional mass transfer model through the packing material for which more complete versions are available.	Good models in search of concepts and actual hydrologic data.	Bounding calculations indicate no problem except hydrologic transport system not well defined. Need to consider modeling of seals.		Second-order plus random sampling techniques potentially powerful. Look forward to application in practice.
TUFF	Location in a favorable environment helps. Dripping of water from unsaturated rock not a credible corrosion scenario.	Incomplete current understanding of complex physical system precludes accurate predictions.	Flow in partially saturated, fractured rock is difficult problem. Appears to have a good technical approach. Can benefit from some work in other areas.	Bounding calculations indicate no problem if estimate of infiltration rate is correct.		Presentation indicates no established methodologies.

radionuclides from all the waste packages and could aid in showing compliance with NRC's release rate criterion. Reliance on a statistical distribution of containment failure times is a major feature in Sweden's KBS-3 repository performance analysis.

For a statistical distribution of containment failure time to be effective, the mean time for failure must be long compared with the radionuclide half-life, or it must be long compared with the allowable mean time for radioactive release, or it must be as long as the time beyond which no calculations of waste-package releases are required. Both canister material and Zircaloy cladding can perhaps be beneficial. For predictive reliability, not only must the expected time of failure be known but also the statistical distribution of failure time. This adds additional challenge to what is already a formidable task: to reliably predict the long-term corrosion and failure of metal containers and fuel cladding.

NNWSI

The assumption of "dripping" of infiltration water in a tuff repository onto waste canisters is unrealistic due to the blotter effect of unsaturated tuff on any water that tries to flow in noncapillaries or in capillaries larger than those in the tuff matrix. During at least the thermal phase, the increased temperature could significantly affect the moisture distribution in the near-field and would likely reduce the apparently small infiltration rate to zero.

NNWSI/LLNL expects major benefit from long-term corrosion resistance of Zircaloy cladding in spent fuel, evidently based upon a compilation of corrosion data by Westinghouse. There appears to be different views within LLNL, PNL (G. McVay, Battelle Pacific Northwest Laboratory, private communication, 1985), Canada (L. Johnson, AECL Whiteshell Nuclear Research Establishment, private communication, 1985), and Sweden concerning the expected corrosion life and failure mechanisms of Zircaloy. For example, LLNL predicts that Zircaloy will last 10,000 years or longer in a tuff repository in the unsaturated zone. Johnson, of Whiteshell, concludes that hydride blistering on the inner surface of partly failed cladding, the resulting delayed stress-corrosion cracking, effects of preemplacement storage, etc., make it difficult to defend the longevity of Zircaloy in granitic ground water. Whereas LLNL emphasizes corrosion in its estimate of Zircaloy life in a repository, other projects conclude that cracking will be the predominant failure mechanism. Potential problem areas of Zircaloy cladding as a barrier due to delayed hydride cracking and stress-corrosion cracking are also emphasized by Rothman (1984). These differences should be resolved.

The tuff project correctly points out that Zircaloy is likely to fail only locally, that even with small penetrations the metal can still present a barrier to radionuclide release, and that a statistical distribution of failure times over the many waste packages in a repository can be of benefit in meeting NRC's release rate requirement. They did not, however, describe a predictive approach that could take these phenomena into account with sufficient predictive reliability, nor did they describe experiments designed to furnish reliable data for such predictions. Developing a plan for accomplishing these would seem worthwhile.

3.2.2 Release Rate Requirement

Section 60.113(a)(1)(ii)(B) of the NRC regulations requires that the release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed 10^{-5}/year of that radionuclide's inventory present at 1000 years after closure. For radionuclides present in small quantities, a different rule applies which implies a release rate of 10^{-8}/year of the total radionuclide inventory (Appendix E).

There are various definitions of the engineered barrier system in the Nuclear Waste Policy Act, the NRC regulations, and the DOE Siting Guidelines. The definition of the engineered barrier system is important in focusing repository design and in relation to compliance with regulations. The differences should be resolved.

The OCRWM Projects should give special consideration to predicting the time-dependent release rates of radium-226 and fission product isotopes such as cesium-137 and strontium-90 to determine if there will be any special difficulties in complying with the NRC release-rate criterion for these radionuclides. Whether the allowable release rate for each of these radionuclides falls under NRC's criterion of 10^{-5}/yr of the 1000-yearinventory of the radionuclide or 10^{-8}/yr times the 1000-year total curie inventory, the problem of meeting the appropriate criterion is affected by the growth or decay of these radionuclides.

The problem with radium-226 arises because the inventory of this radionuclide grows continuously from the time the waste is emplaced in the repository. Its inventory at 10,000 years is about 50 times greater than its 1000-year inventory. If the required technical performance of a waste form-engineered barrier system is to be expressed as the allowable instantaneous fractional release rate of a contained species (i.e., the actual release rate at some time normalized to the instantaneous inventory of that species at that time), then ingrowth of radium-226 with time will require an instantaneous fractional release rate at 10,000 years that is 50 times lower than the allowable fractional release rate based on its 1,000-year inventory. This emphasizes the importance of the phenomena controlling radium-226 release from the waste package the longer the waste resides in the repository.

It may be difficult to demonstrate sufficiently low release rate of radium-226 for a waste package surrounded by thick backfill, with assumed saturation concentration of radium and its precursors at the inner surface of the backfill, as in the BWIP release-rate calculations. Depending upon the retardation parameters, decay of uranium-234 and thorium-230 while in the backfill can lead to higher local concentrations and release rates of radium-226 at the backfill-rock interface than would be experienced at the inner surface of the backfill. This should be calculated. To meet the release-rate criterion for radium-226 it may be necessary to rely upon the slow rate of reaction of water with the waste form, upon release barriers in partly failed cladding and canisters, or upon statistical failure distributed over many packages.

The problem with cesium-137 and strontium-90 arises if waste-package containers are expected to fail extensively after only a few hundred years. For example, the inventory of cesium-137 is appreciable during the first few hundred years of emplacement. For a given allowable curie release rate of cesium-137 under the NRC release-rate criterion, the allowable fractional release rate of cesium-137 after a few hundred years of emplacement, which is the ratio of the allowable curie release rate divided by the instantaneous inventory of cesium-137 at the time it is being released, can be very low. To illustrate, in a repository loaded with waste from 70,000 metric tons of reactor-fuel uranium, the inventory of cesium-137 at 1,000 years is expected to be 0.6 curie. The total curie inventory of radionuclides at 1,000 years is about 1.1×10^8 curies, and the NRC alternate criterion would allow a maximum release rate of 1.1 curies/year at any time for any radionuclide including cesium-137. Thus, the allowable annual fractional release for cesium-137 at 1,000 years is greater than the inventory at that time. However, if the waste form is exposed to ground water as early as 300 years, the earliest time allowable under NRC regulations, the cesium-137 inventory at that time will be 6×10^6 curies, and the allowable fractional release rate of cesium at 300 years will be 2×10^{-7} per year, based on its inventory at that time. This could be a formidable requirement in some repository designs, if all waste forms were exposed to ground water at 300 years and if there were no appreciable time delay for dissolved cesium to reach the outer edge of the engineered barrier system. In this case, a more detailed but realistic analysis of waste package releases would be necessary.

It was reported to PANRG that some projects are estimating the source term at the surface of the waste package by assuming concentrations related to mineral solubilities obtained from handbooks or the WISP report (Pigford et al., 1983). In actual repository environments, the minerals present will limit maximum possible concentrations of the radionuclide. If the specific solid phases, including minerals, formed by waste package-water-rock reactions are known, and if suitable thermodynamic data exist, then computer programs such as WATEQF (Plummer et al., 1976) and EQ3/EQ6 (Wolery, 1979; 1983) can assist in the calculations. Currently, the best thermodynamic data available, and thus the best predictions that can be made are probably for iodine, lead, radium, strontium, thorium, and uranium. A second and complementary approach to defining the source term is to perform solubility experiments designed to duplicate anticipated water-rock conditions adjacent to the waste. Such experiments can serve to verify the solubilities predicted through computer modeling, or serve as the basis for predicting source term concentrations for radionuclides when the thermodynamic data needed for model calculations are inadequate. It is our understanding that such solubility experiments are being performed by the basalt project and are planned by the tuff project.

<u>BWIP</u>

In addition to a uniform corrosion model, BWIP presented a one-dimensional analytical model that predicts the transport of radionuclides through the bentonite/basalt packing material and into the host rock. The basalt project represents the waste package by an infinite planar surface, packing material by a semi-infinite slab, and rock by an infinite half space.

Separate numerical calculations show that the ground-water velocity through the packing material is low enough to neglect advection in the mass-transfer calculation. Assuming saturation concentrations of each waste constituent at the inner surface of the packing material, they calculate the time-dependent rate of release of individual radionuclides from the packing material into the rock. BWIP is conducting hydrothermal experiments with waste samples in simulated ground water to determine the effective saturation concentrations to use in this calculation.

The mass-transfer approach for estimating dissolution rates and release rates of individual radioelements was recommended by the WISP report for situations in which waste packages are surrounded by ground water in porous or fractured rock. The mass-transfer approach is the mainstay of the KBS repository design and performance analysis, and it provides a predictive technique for calculating the lifetime of the copper canister as well as a technique for calculating dissolution rates and release rates of radioelements.

BWIP's planar-geometry model may be producing reasonable estimates of the maximum release rate, but further validation is necessary. A planar- geometry backfill adjacent to an infinite half-space of rock, with no radioactive decay and negligible advection, will not yield a steady-state solution. It will predict release rates that approach zero at long times, a result not expected on physical grounds. A finite rate at steady state is expected and is predicted by the more realistic models of Chambre' et al. (1983, 1984). These models treat the waste form as cylindrical and spherical equivalents and include radioactive decay which is important for some strongly sorbing radionuclides diffusing through the packing materials. Also, Chambre's analytical solutions for diffusion-advection mass transfer, together with the solution for diffusion-controlled mass transfer, provide a clear mathematical criterion to determine when effects of advection can be neglected in mass-transfer calculations.

For its mass transfer analysis, the basalt project conservatively assumes that all waste constituents are at their saturation concentrations at the inner surface of the backfill, resulting in predicted release rates for some of the more soluble constituents that are greater than may be considered acceptable. The recent analytical solution of Zavoshy et al. (1984) could help BWIP in estimating more realistic and less conservative release rates for these constituents. This solution predicts the concentration of a waste constituent at the inner surface of the packing material by using experimentally determined rates of forward reaction between ground water and the waste solid and measured saturation concentrations, rather than assuming saturation.

It is understood that BWIP's calculations of mass transfer from the waste package have assumed ambient isothermal conditions. Because of the very long time of the thermal period in a basalt repository, it would seem desirable to estimate the effect of time-dependent temperatures on mass transfer, if the heats of solution or temperature-dependent solubilities are known. Chambre's analytical solutions (Chambre' and Pigford, 1984; Chambre' et al., 1984) for temperature-dependent diffusion from waste into rock could be useful.

NNWSI

NNWSI/LLNL concludes that the NRC 10^{-5}/yr release-rate requirement can be met at the waste package, based on a bounding calculation that assumes that all of the water flowing through the repository becomes saturated with silica from glass waste or uranium dioxide from spent fuel. Only this general conclusion was stated; no calculated results for radionuclides were presented. No values of solubilities used in these calculations were provided. NNWSI/LLNL assumed that constituents other than the waste matrix dissolve congruently with the matrix. However, congruent dissolution is not expected, for reasons outlined in the WISP report (Chapter 5), and the NNWSI/LLNL assumption is not necessarily conservative or bounding.

NNWSI/LLNL qualitatively described plans for experiments intended to aid in predicting the long-term release rates of radionuclides from spent fuel and glass waste in a tuff repository. These will be real-time laboratory experiments, such as dripping ground water on a composite waste package. LLNL described the physical and chemical processes that they expect to study, but there is evidently no plan now as to how these real-time laboratory data can be used to predict long-term performance in a repository. NNWSI/LLNL may not be able to observe radionuclide releases during the time-scale of their experiments. If finite releases are observed, the observed rate constants are not likely to be representative of rates that would be expected during several millenia in a repository.

The experiments described by NNWSI/LLNL to observe releases and release rates appear to be typical of laboratory screening experiments. Such experiments are useful when the mechanisms of release are not well known, but without guidance from a predictive technique or theory applicable to the repository environment the resulting real-time data cannot be expected to provide a basis for quantitative predictive reliability. A qualitatively similar approach was followed for over a decade in laboratory leach measurements of the leach rate for borosilicate glass and other waste forms, where careful experiments have yielded files of test data but without an adequate correlative technique for radionuclide release during the real time of laboratory experiments and without a reliable way of applying these data to predicting long-term radionuclide release rates in a repository (WISP report, Chapter 5).

Consideration should be given to the pitfalls that can result from extensive laboratory screening experiments without early concentration on what data are needed for reliable quantitative prediction of long-term performance in a repository environment. Mass-transfer analysis, i.e., the detailed examination and quantification of the rate processes that control interphase transfer of material, should be applied to predicting release rates in a tuff repository and to the design of experiments to yield data necessary for reliable and quantitative prediction.

SRP

The salt project estimates radionuclides release rates from the waste package by calculating the time-dependent migration of brine inclusions into the waste-package cavity and by assuming that the accumulated brine is always saturated with individual waste constituents. If this very conservative approach is sufficient to demonstrate compliance with NRC's release-rate criterion, then a more realistic approach may be unnecessary.

The above approach, however unrealistic, requires reliable data on solubilities and reliable estimates of thermally induced migration rates of brine inclusions. Although the brine-migration predictions by the Jenks model (Jenks and Claiborne, 1981) are thought to be conservative, this approach remains somewhat uncertain. The Jenks model assumes that inclusions migrate from one halite crystal into adjacent crystals, crossing grain boundaries in the process, until the inclusions finally reach the waste-package cavity (if a cavity still exists). It is believed that inclusions probably follow a pathway along grain boundaries after they have left the halite crystal in which they originally reside. The mathematics and controlling parameters for this process are not the same as for the model adopted by Jenks. Results from newer predictions of transport via grain-boundaries were described briefly by SRP, but it appears that these newer predictive models have not been evaluated or tested.

3.2.3 Travel Time Requirement

The NRC requirement is that the pre-waste-emplacement ground-water travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1000 years (Section 60.113(a)(2)). A clarification of how to show compliance with this requirement is needed.

The basalt project used Monte Carlo simulation to derive travel times. The tuff project has a very difficult problem of predicting travel time in an unsaturated zone. In the salt project, the definition of the disturbed zone is essential to the calculation of travel time and needs clarification.

As discussed under Technical Observations Nos. 1 & 8 in Section 3.1, serious problems exist in the NRC requirements. In addition to the basic problem of the definition of travel time itself, serious questions exist concerning the strict application of the travel-time criterion for exclusion of potential repository sites. Specifically, if the ground-water flux approaches zero, the potential mean flux of radionuclides also must approach zero. Although a small amount of water may travel through the repository and hence to the accessible environment in a very few years, the total amount of radionuclides which are transported might well be insignificant. In general, the PANRG has the impression that too much attention has been paid to water travel time with insufficient consideration of the actual ground-water flux which will significantly affect radionuclear transport, particularly of radionuclides having long half-lives.

BWIP

Differences of opinion between the project and the U.S. Geological Survey regarding geohydrologic conditions at the BWIP site were noted, as were activities undertaken to resolve these differences. There was no extensive discussion of the issues involved, but the issues must be clearly delineated and the requirements for their resolution be mutually understood as well. Such resolution should involve a cooperative effort by the organizations involved.

The only geohydrologic flow model discussed was a two-dimensional "flow top" model. Probabilistic results were obtained using a stochastic treatment of transmissivity, but with a fixed effective thickness and regional hydraulic gradient. More detailed or sophisticated multivariate analysis was limited by lack of data. In future analyses of the latter kind, consideration should be given to the validity of sampling transmissivity and effective-thickness distributions since both are affected by aquifer thickness.

The effort to include "fracture effects" in the flow model studies may perhaps be an unnecessary over-complication. Factors related to fractures such as flow capacity, frequency, orientation, continuity, etc., will have to be defined, and the fracture "system" will need to be modeled accordingly. A major effort to develop fracture models might be deferred until shafts and drifts are available for direct measurements of the hydraulic properties of permeable fractures.

NNWSI

Travel time from the repository to the water table is highly dependent on infiltration rates, with the travel time changing by several orders of magnitude as the infiltration rate changes from 0.1 to 1 mm/year. A dynamic model which accounts for changes in water storage within the unsaturated media would permit assessment of the impact of slight or slow changes in climate on the water travel time. Also, to test whether or not such changes have occurred in the past, investigation of natural radionuclides in the pore water at the repository horizon should be carried out.

The tuff project presented a discussion of rather sophisticated three-dimensional flow and transport equations relative to flow in fractures and the matrix in unsaturated porous media. However, good approaches to estimating dispersion coefficients in unsaturated rock media are lacking. As noted in Chapter 4, Section 4.1, the estimation of dispersion coefficients in saturated media is an art, and it is a developing art in unsaturated rock (Yeh and Gelhar, 1983).

The results of the system study which were presented were based on the SPARTAN code which assumes plug flow. Comparison with similar results using the TOSPAC code (which includes dispersion) would help to evaluate the importance of dispersion.

SRP

The salt project has calculated the time required for brine diffusion to transport radionuclides through the salt. In this approach, the key is the derivation of a "brine diffusion coefficient" obtained from field data on water content versus distance from a sediment inclusion. The diffusion coefficient obtained from such a calculation obviously depends on the assumption of the starting time of the diffusional process. This is not a sufficient basis; additional field data of this type should be sought to validate the diffusion parameter.

The salt project presented details of elaborate modeling of regional hydrology (Gupta, Cole, Bond and Monti, 1984). While such modeling would be important for some purposes, very detailed analyses and calculations of the flow field in the formations adjacent to the salt would be significant only if a salt repository is breached. Given the nature of potential salt sites, only reasonably approximate models of the flow in the adjacent formations are needed. A particular problem for salt repositories is that there is no generally accepted definition of the boundary of the disturbed zone from which the ground-water travel time to the accessible environment is to be determined. Priority attention might be addressed to confirming whether or not the salt can be breached at the sites involved (Chaturvedi and Rehfeldt, 1984).

3.2.4 Cumulative Release Requirement

Most of the results presented to us on compliance with the EPA standard were of the "bounding calculations" variety.

BWIP

The basalt project presented selected results from the stochastic systems model EPASTAT, which calculates the projected releases at the accessible environment using random sampling of key parameters. With appropriate data, the EPASTAT model can be a credible approach to showing compliance with the EPA standard.

Briefings on the major geohydrologic models developed by BWIP (i.e., PORFLO and MAGNUM) were specifically requested but were not provided. Thus, we cannot comment on the adequacy of their approach or their work in geochemical retardation. Requested briefings on their approach to modeling resaturation and seals and plugs also were not provided.

NNWSI

The tuff project is still developing their understanding of flow and transport processes in the unsaturated zone at Yucca Mountain. The PANRG observes that the modeling of flow and transport through partially saturated, fractured rock is perhaps the most difficult problem in performance assessment.

Based on information presented to PANRG, efforts are being made by NNWSI to assess the magnitude of and variation in the water saturation or moisture content above the water table in the tuff indirectly through the use of laboratory psychrometric tests developed and used widely by soil scientists. Presumably, it is intended to check these values against those obtained by more direct measurements on cores recovered from wells or from the interpretation of well logs. Suggestions pertinent to these latter direct methods are presented in Section 4.4 of this report. There are additional indirect methods described in the literature; i.e., mercury injection or centrifuge (Wardlaw and Taylor, 1976; Hassler and Brunner, 1945; Hoffman, 1963) for studying capillary pressure and pore structure of porous media that can provide results similar to those obtained by psychrometric methods. These methods take considerably less time and perhaps should be considered by NNWSI if they have not already done so.

Once the variation of moisture content with depth is known, then it is our understanding that NNWSI will use empirically determined relationships to relate water conductivity with initial partial water saturation or moisture content. For example, in the TRACR3D code, one of the codes NNWSI is using for three-dimensional unsaturated flow in porous media, the Brooks-Corey (1964) relationship is used (Travis, 1984). We understand that in other NNWSI unsaturated flow codes, a relationship by Mualem (1976) is used. In their presentations, NNWSI revealed that they were not aware of experimental procedures that had been developed within the oil industry for making such measurements on low conductivity porous media. Such experimental measurements on a few tuff samples would allow adjustment, if needed, of their calculational procedures and thus provide initial water and air flow conductivities more representative of actual conditions.

The TRACR3D documentation volume indicates that the same calculational procedures would be used to describe the water and gas conductivities as tuff water saturations increased (due to surface moisture drainage vertically downward). Account must be made in such calculations for the hysteresis that occurs in both capillary and conductivity relationships when the water saturation increases. Experimental data available in oil industry literature (Geffen et al., 1952; Colonna, Brissaud and Millet, 1972; Schneider and Owens, 1976; Killough, 1976) indicate that for systems that are preferentially water wet (which the tuff should be), the conductivity to water is little affected by the direction of water saturation change (i.e. increasing or decreasing). However, there is a significant effect on gas phase conductivity and thus the transport of radionuclides that would exist in a gaseous phase. As the water saturation increases from some initial value, gas conductivity quickly drops to zero as the gas saturation becomes "trapped" by the increasing water saturation. It is a very complex situation since the relative gas conductivity and the "trapped" gas saturation are functions of the magnitude of the initial gas saturation. Laboratory measurements of this type on tuff samples can perhaps be arranged with one of the oil service companies (Core Laboratories, Inc., Dallas) to provide a basis for calibrating or adjusting calculational procedures used in the performance assessment codes.

In a repository in unsaturated tuff, the heat from the waste packages will create a complex flow regime of steam, air and water. The same phenomenon will exist at BWIP during resaturation. BWIP and NNWSI did not present a model that will handle two-phase, two-component flow although we understand that such codes exist.

In view of the complexity of multiphase flow near a repository, it seems desirable to review the physics of the entire hydrologic model for a repository in tuff considering (1) the initial water saturation and flow condition, (2) changes in saturation and flow of both water and air as water saturation increases due to water movement downward from the surface, and (3) changes in saturation and flow of both water and air due to the heating of the rock surrounding the waste packages.

In terms of radionuclide transport, the tuff project assumed that water saturation conditions existed, and that there would be no retardation of iodine-129 or carbon-14. Goldberg et al. (1962) measured the adsorption of iodine-131 on ground Rainier tuff and obtained a distribution coefficient (K_d) of about 1 ml/g. This suggests iodine retardation by a factor of 5 to 11 times (Freeze and Cherry, 1979). Ames and Rai (1978) pointed out that iodide sorption by low pH soils (4 to 6) can be almost complete, with K_d values up to 50 ml/g. Assuming that carbon-14 is not retarded is also questionable because carbon-14 is likely to be partially retarded by calcite precipitation in the tuff and by isotopic exchange.

SRP

The salt project presented several approaches to show compliance with the EPA standard. First, they used the intrusion scenario suggested in Appendix B of Draft No. 4 of the proposed EPA standard (USEPA, 1984a). They also presented parameter variation analyses of one particular intrusion scenario. If SRP's interpretation of how to show compliance with the EPA cumulative release limit is correct, then their calculations of radionuclide diffusion showed that they comply. Combined with the understanding that the normal scenario of a repository in salt gives zero release, the salt project appears to have the methodology to show compliance with the cumulative release limit in the proposed EPA standard.

The PANRG noted that modeling of ground water flow in the regions overlying a salt repository is well established and that transport of radionuclides from a hypothetically breached salt repository can be adequately predicted if the rate of radionuclide release from the fuel packages is known (Pearson et al., 1983). Further development of regional ground water flow models may not be needed, but these models should be used to produce radionuclide transport results that are now lacking.

Existing knowledge of the chemistry of brines from bedded salt and salt domes has not been fully utilized in studies of possible mass transport in these materials. For example, the salt project assumes fixed pH's and oxidation-reduction potential and brine compositions which do not take into account the effect of temperature on salt and other mineral solubilities. In response to a question as to how it was intended to validate the assumed solubility limits used in the source term, it was stated that they would compare and adjust the assumed solubilities as needed based on radionuclide solubility measurements in Salton Sea brines. Solubilities would be modeled using a modified EQ3/EQ6 computer program with high ionic strength capabilities based on a Pitzer-type modelling approach (Harvie and Weare, 1980). Why use a Salton Sea brine? Why not measure and model radionuclide solubilities in brines having the basic composition of those in the salt formations? The Salton Sea is a surface water and, unless stratified, will be aerobic. Brines in the salt formations are largely anaerobic. The solubilities of radionuclides such as uranium, plutonium, neptunium, iodine and selenium are strongly oxidation-reduction potential dependent, and can differ by 10 times or more depending on oxidation-reduction potential of the brine.

The salt project did not respond to the request for a presentation on modeling of seals and plugs.

3.2.5 Uncertainty Analysis

The values of parameters used in performance assessment are often quite uncertain and may range over several orders of magnitude. The necessity of acceptable methodologies for handling uncertainties is recognized, and the NRC has emphasized the need for formal, detailed analyses to support the licensing process.

The PANRG requested that the Projects provide briefings on their uncertainty analysis approaches and available results. Our main conclusions were the following:

- There is uneven development of techniques among the Projects.
- The techniques developed by one project can also be used by others.
- BWIP and SRP have developed approaches to uncertainty analysis which seem appropriate. This will be better confirmed when actual results become available.

BWIP

The basalt project uses random sampling or Monte Carlo for uncertainty analysis. Random sampling is a well-established form of uncertainty analysis, but large amounts of computation time are required. BWIP uses a second-order sensitivity analysis approach (Sagar and Clifton, 1983). The second-order analysis approach solves the relevant stochastic differential equations of ground-water flow using a second-order Taylor series expansion of the variables around their means. The basalt project is experimenting with this approach, and it appears to show promise.

NNWSI

The tuff project is still developing its understanding of geologic and hydrologic processes in the unsaturated zone and proposes using the random sampling approach for uncertainty analysis.

SRP

The salt project uses a combination of random sampling and adjoint sensitivity analysis for its regional ground-water flow models. In contrast to the second-order method used by BWIP, the adjoint method is a first-order Taylor series expansion around the means of the uncertain variables (INTERA, 1983b). The adjoint method is well known in the nuclear engineering field and is becoming popular in general ground-water and thermo-mechanical analysis. SRP has also developed a code that will operate on any other code that numerically solves partial differential equations, and provide adjoint sensitivities.

These methods appear powerful and potentially useful to all the Projects. However, the PANRG cannot judge the adequacy of these methods without seeing actual results.

CHAPTER 4

TOPICAL REVIEWS

In this chapter, the Performance Assessment National Review Group offers additional detailed comments on selected topics.

4.1 Dispersion and Stochastic Hydrology

Should radionuclides be released from an underground repository of nuclear waste, then the primary mechanism for transporting and spreading them will be ground-water movement. The degree to which a plume of radionuclide spreads is a function of both the flow field and dispersion. A number of Project presentations have expressed uncertainties in regard to the modeling of hydrodynamic dispersion as a transport mechanism. Among the questions discussed were the relative importance of dispersion vis a vis advection, adsorption, and decay; the validity of the dispersive transport equations based on Fickian transport laws; and the advantages and disadvantages of deterministic and stochastic approaches to the modeling of dispersion. The purpose of this short review is to give a brief introduction to the modeling of hydrodynamic dispersion phenomena in porous media to provide a common basis for further discussion of this problem within and among the Projects.

4.1.1 Dispersion in Homogeneous and Isotropic Porous Media

Figure 4.1 shows two examples of the dispersion phenomena. For simplicity, it will be assumed that the porous media is fully saturated and consists of a closely packed assemblage of identical solid grains; therefore, the porous media is both homogeneous and isotropic in structure. Initially, a tracer-labeled liquid occupies the region to the left of an interface, separating it from an unlabeled liquid as shown in Figure 4.1(a). As flow takes place, the interface does not remain abrupt; however, its mean position is determined by a spatially averaged advective velocity (i.e., the pore velocity given by the Darcy velocity divided by the porosity). In time, the initially abrupt interface is replaced by an ever-widening transition zone across which the tracer concentration varies from that of the tracer liquid to that of the unmarked liquid. In order to describe this phenomenon in terms of classical transport theory, we normally invoke the concepts of advective and diffusive fluxes. The former is expressed in terms of the product of tracer concentration and pore velocity, while the latter is given by the product of the molecular diffusivity of the tracer and its longitudinal concentration gradient. The diffusive flux would cause a spreading of the initially abrupt interface even in the absence of any flow. However, it is well known that when an advective flow is present, the width of the transition zone is such that a diffusion coefficient many orders of magnitude larger than the molecular diffusivity may be required. The additional spreading, which is related to the flow, is caused by non-uniform velocity distributions within the intergranular passages and by the multitude of tortuous flow passages through the assemblage of solid particles. Both effects contribute to the

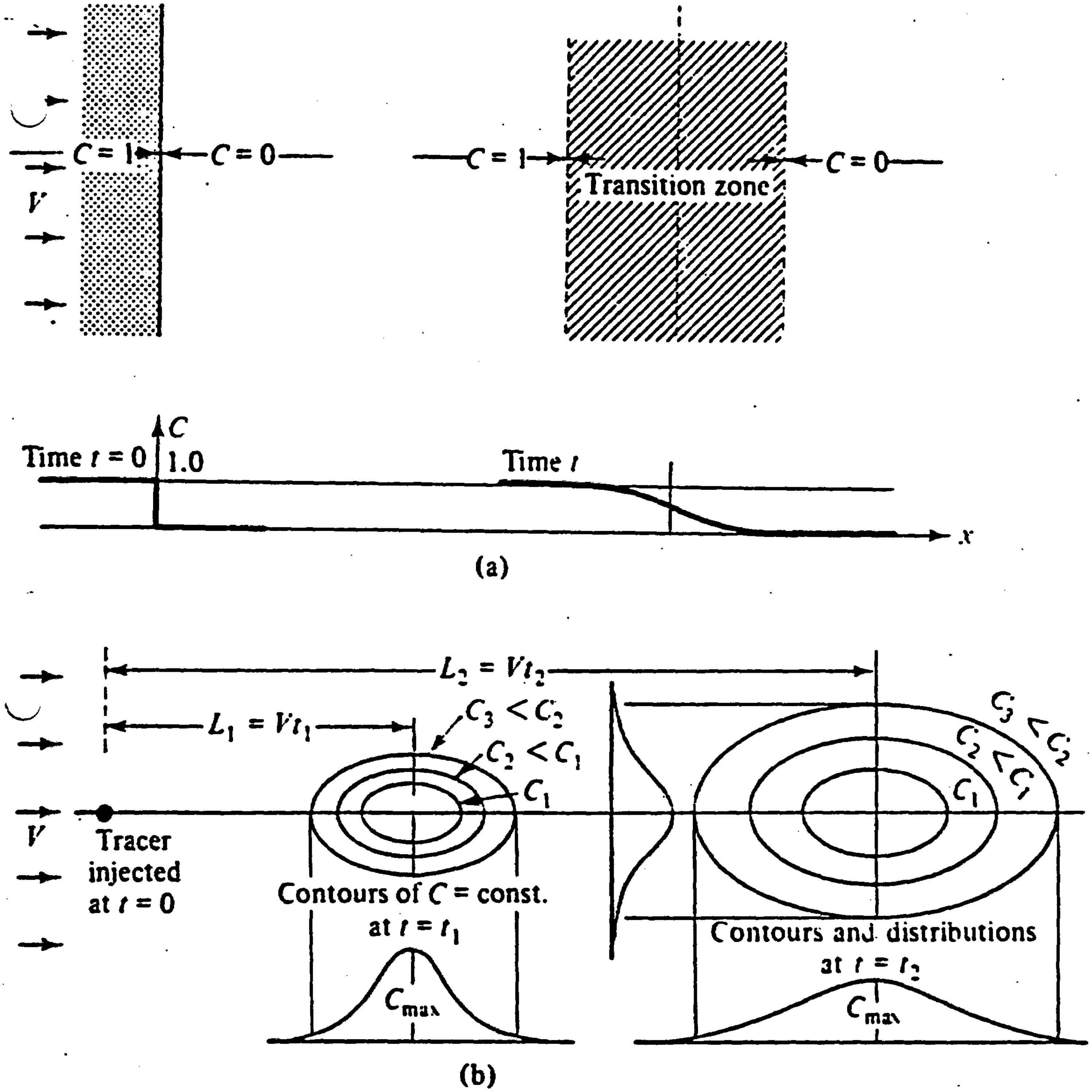

Figure 4.1 Longitudinal and Transversal Spreading of a Tracer.
(a) Longitudinal Spreading of an Initially Sharp Front.
(b) Spreading of a Point Injection. Source: Bear (1979).

spatial variability of the velocity at the microscopic level. None of this velocity variability is captured by the average pore velocity (which by definition is a velocity averaged over a macroscopic volume much larger than a single grain); therefore, the additional spreading caused by the microscopically non-uniform spatial velocity must be accounted for by adding a "mechanical dispersion" term to the molecular diffusivity. Thus, the total or hydrodynamic longitudinal dispersion coefficient D_L is defined as the sum of the mechanical dispersion D_m and the molecular diffusivity D^*

$$D_L = D_m + D^* \tag{1}$$

The advective - dispersive mass transport equation for a conservative substance is

$$\frac{\partial c}{\partial t} = (\nabla \cdot D\nabla - \nabla \cdot \underline{v})c \;;\; c(\underline{x},o) = c_o(\underline{x}) \tag{2}$$

where c is the concentration of the tracer, $\underline{x}$ is the position vector, t is time, D is the hydrodynamic dispersion tensor, $\underline{v}(\underline{x})$ is the pore velocity vector, and ∇ the gradient operator. The general assumption is that the dispersive mass flux, J_d, follows Fick's first law,

$$J_d = - D\nabla c$$

The dispersive effect is of interest because it results in the arrival of the contaminant at a discharge point or arbitrary boundary prior to the arrival time that would be calculated from the spatially averaged pore velocity. It is also seen that the prediction of the concentration of dispersed tracer or radionuclide depends heavily on the ability to calculate the dispersion tensor.

Another example illustrating the multi-dimensional nature of dispersion is that of an instantaneous injection of a tracer at a point in a porous medium with a uniform flow as shown in Figure 4.1(b). The sketch illustrates the dispersion resulting from longitudinal and transversal (to the flow direction) spreading. In the three-dimensional case, the relationship between the dispersion due to the porous matrix geometry and the flow velocity is given by (Bear and Bachmat, 1967)

$$D_{ij} = a_{ijkm} \frac{V_k V_m}{V} \tag{3}$$

where V is the pore velocity and a_{ijkm} is a tensor having the dimensions of a length called the geometrical dispersivity (molecular diffusion is neglected). In an isotropic porous medium, a_{ijkm} is related to two constants, a_L and a_T, representing the longitudinal and lateral dispersivities, thus

$$D_{ij} = a_T V \delta_{ij} + (a_L - a_T) V_i V_j / V \tag{4}$$

where δ_{ij} is the Kronecker delta. In Cartesian coordinates, the hydrodynamic dispersion tensor D_{ij} has nine components, three of which D_{xx}, D_{yy}, D_{zz} are along the principal axes, and the remaining six are diagonal (e.g., D_{xy}). If the pore velocity is unidirectional, uniform, and oriented along the x axis, the diagonal terms disappear and equation (4) reduces to coefficients of longitudinal and transverse dispersion,

$$\begin{aligned} D_{xx} &= D_L = a_L V \\ D_{yy} &= D_{zz} = D_T = a_T V \end{aligned} \tag{5}$$

If a Cartesian coordinate system is aligned so that the average uniform velocity is along one of the axes, say x_1, then we can write the dispersion tensor in matrix form as

$$D = \begin{bmatrix} a_L V & o & o \\ o & a_T V & o \\ o & o & a_T V \end{bmatrix}$$

or

$$D = \underline{A} V$$

where $\underline{A}$ is now a matrix of dispersivities or the effective dispersivity tensor. We shall see later how stochastic theory leads to the specification of $\underline{A}$.

Many laboratory experiments on longitudinal and lateral dispersion in isotropic media have been carried out, and a number of these indicate that the dispersion coefficients are not exactly linear functions of the pore velocity as indicated by equation (5). For example, Harleman, Mehlhorn and Rumer (1962) found that the longitudinal and lateral dispersion coefficients are approximately,

$$\begin{aligned} D_L &= d\, v^{1.2} \\ D_T &= \frac{d}{50} v^{0.6} \end{aligned} \tag{6}$$

where d is the diameter of the uniform grains.

Attempts to apply this model to large-scale laboratory and field tracer experiments have led to several difficulties. One difficulty is that a_L and a_T seem to vary with the scale of the experiment. Whereas in the laboratory a_L ranges from 10^{-4}m to 10^{-1}m for relatively uniform fine - to coarse-gained soils and up to almost 1 m for coarse gravel (Bear, 1961; Lawson and Elrick, 1972; Koltz et al., 1980); in field tracer experiments, a_L varies from 10^{-2}m to 10m, and on occasion may exceed 10^2m (Lallemand-Barres and Peaudecerf, 1978; Anderson, 1979; Pickens and Grisak, 1981). When a_L is obtained by matching the output of computer models based on (2) with documented histories of aquifer pollution on a regional scale, its value ranges from less than 10 m to more than 100 m (Anderson, 1979). Another difficulty is that, in a given tracer experiment, a_L and a_T appear to grow with distance of the sampling point from the source (Martin, 1971; Lawson and Elrick, 1972; Peaudecerf and Sauty, 1978; Sudicky and Cherry, 1979; Sudicky et al., 1983; Dieulin et al., 1980; Silliman and Simpson, 1983). In fact, disregarding this phenomenon and treating a_L as a constant may lead to the physically unacceptable conclusion that a concentration plume could spread upstream at a rate exceeding that predicted by molecular diffusion alone (de Marsily, 1978; Simpson, 1978). Later, some results from stochastic analysis can be shown to circumvent the problem.

4.1.2 Dispersion in Heterogeneous Porous Media

An aquifer composed of heterogeneous unconsolidated deposits in which the heterogeneities occur as layers or beds of different hydraulic conductivity is shown in Figure 4.2. The ground-water flow is assumed to be parallel to the bedding planes. Contaminants introduced by advection would be transported at different rates in each layer in accordance with the differences in their hydraulic conductivities. Thus, in the absence of interaction between the layers, advective transport in the stratified system would result in large spatial variations in the contaminant distribution. As discussed in the previous section, the effect of the molecular diffusive and microscopic intergranular flows known as transverse dispersion would be to transport mass laterally and smooth out the transverse concentration gradients. In the longitudinal direction within a high-permeability layer, the centroid of a tracer slug moves forward at a rate slower than the pore velocity in the layer because mass is lost from the layer by lateral transfer. Similarly, in the longitudinal direction within the lower-permeability layer, the front of the slug moves faster than its pore velocity because these layers are continually acquiring mass from the adjacent, more permeable layers.

A discussion of transport in layered media is a useful exercise because various researchers have used this aquifer geometry to demonstrate (1) non-Fickian behavior and scale effect (i.e., increasing dispersivity with size of the plume) and (2) stochastic modeling techniques.

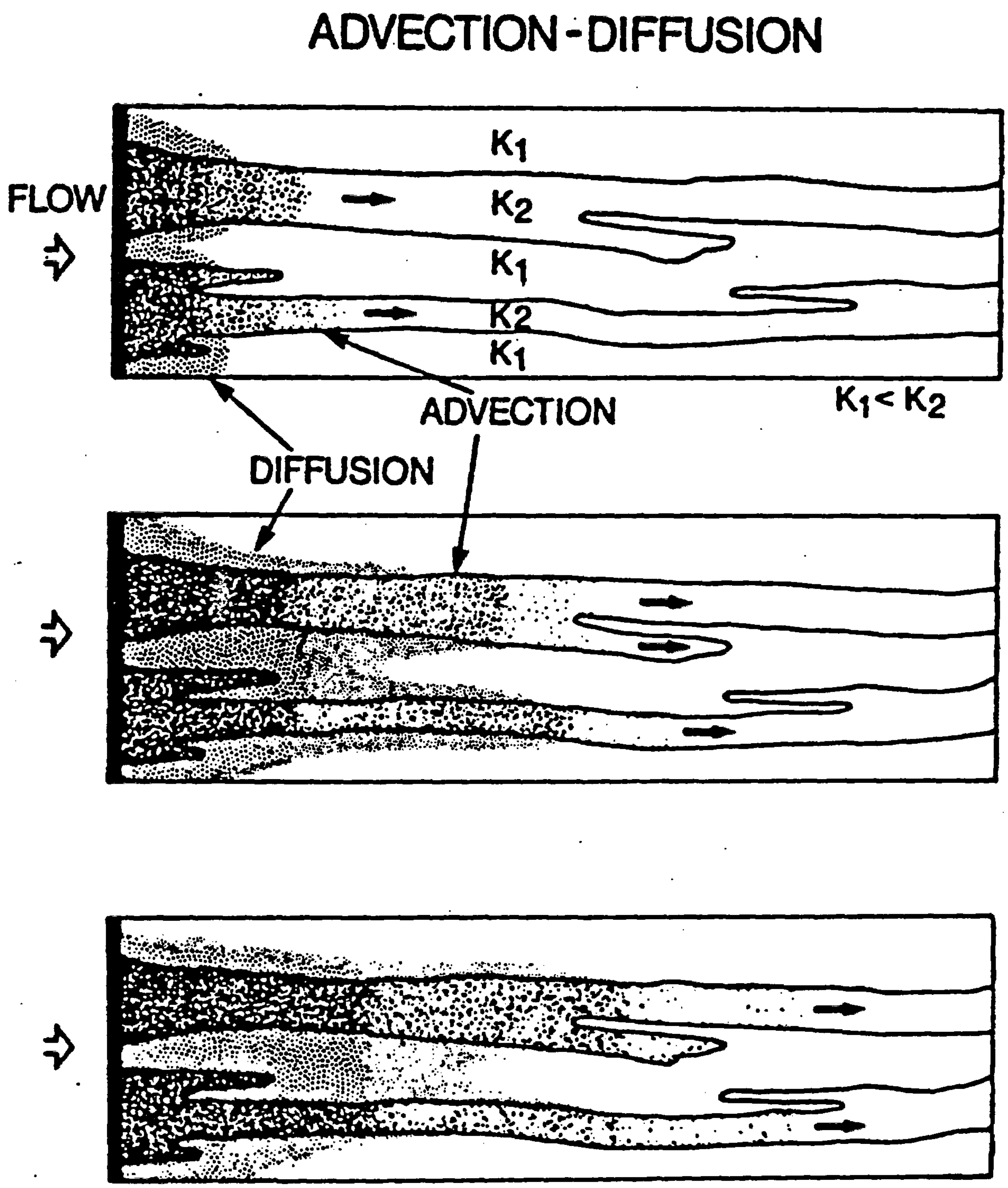

Figure 4.2 Schematic Representation of the Advection-Diffusion Process. Source: Gillham et al. (1984).

4.1.2.1 Validity of the Fickian Dispersion Relationship

A number of researchers have questioned the validity of G.I. Taylor's demonstration that dispersion could be represented as a Fickian process. An example is the study by Gillham et al. (1984) shown in Figure 4.3(a), of flow in a single, high-permeability layer embedded in a non-flowing, low-permeability region. A slug of tracer is introduced instantaneously into the high-permeability layer (Figure 4.3(b)) and is assumed to be advected along this layer at a rate equal to the layer-averaged pore velocity. Hydrodynamic dispersion in the longitudinal direction is neglected, and mass is assumed to be transported laterally only under the action of molecular diffusion.

The calculated spatial concentration distributions at 5, 10, and 15 days are shown in Figures 4.3(c) and 4.3(d). These skewed distributions depart from the Gaussian distributions that would be predicted from the Fickian relationships. The authors also present a plot (Figure 4.4) of the calculated spatial variance σ_x^2 versus time to show that this is not in accord with classical dispersion theory in which the time rate of change of the variance is related to the longitudinal dispersion coefficient by

$$\frac{d}{dt}(\sigma_x^2) = 2D_L \qquad (7)$$

Equation (7) implies that if D_L is to be a constant, σ_x^2 should be linear in t. However, Figure 4.4 indicates that as time increases, the variance increases in a non-linear manner and, therefore, the longitudinal dispersion coefficient increases. Nevertheless, the time rate of change of the variance appears to approach linearity at large times, implying that, after an initial development period, the dispersion process becomes Fickian. Taylor and others who continued the development of the theory of dispersion clearly recognized that the Fickian assumption was not valid at early times or within small distances from the source. An objection to the Gillham et al. (1984) analysis, which probably exaggerates the non-Fickian behavior, is the neglect of longitudinal dispersion. This term is important for a pulse injection because of the large second derivative of the longitudinal concentration distribution. If included, this effect would probably decrease the time or distance required to approach Fickian behavior. A number of researchers estimate that distances from tens to hundreds of meters are required for the zone of initial development (Matheron and de Marsily, 1980; Gelhar and Axness, 1983; Dagan, 1982).

Marle et al. (1967) treated a stratified (heterogeneous) aquifer with flow parallel to the bedding planes in a medium with finite vertical thickness. The variation of hydraulic conductivity in the vertical direction is handled by assuming the local horizontal pore velocity u to be a given

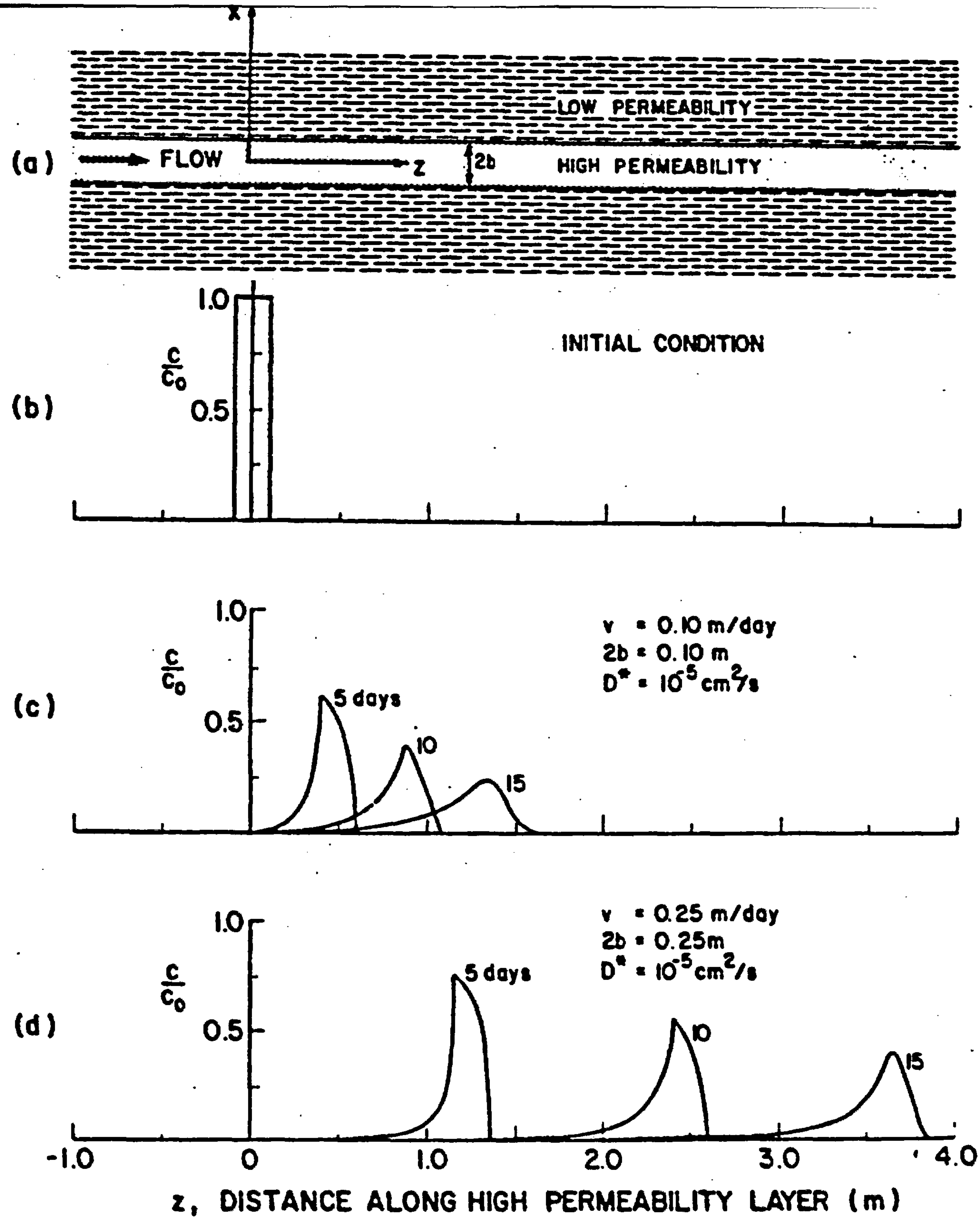

Figure 4.3 Single-Layer Advection-Diffusion Model. (a) Physical System. (b) Initial Conditions. (c) Concentration Profiles for v = 0.10 m/d and 2b = 0.1 m. (d) Concentration Profile for v = 0.25 m/d and 2b = 0.25 m. Source: Gillham et al.(1984).

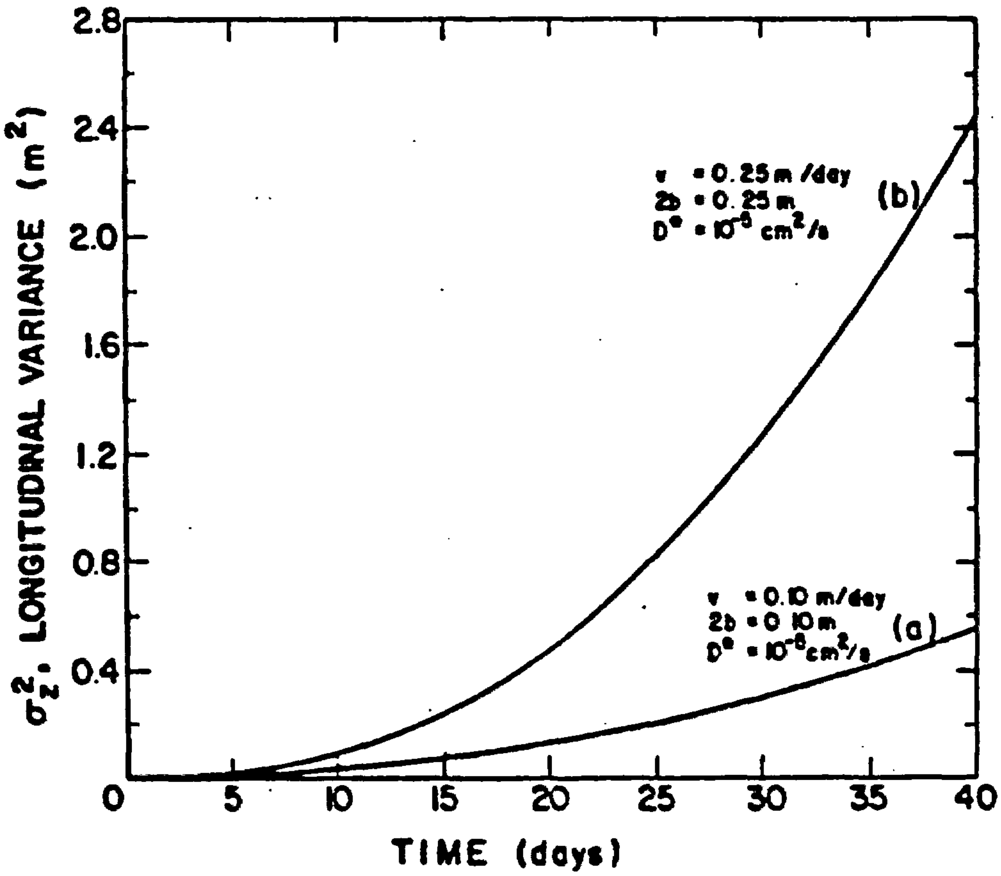

Figure 4.4 Longitudinal Variance of Concentrations Versus Time for the Single-Layer Model: (a) v = 0.10 m/d and 2b = 0.10 m. (b) v = 0.25 m/d and 2b = 0.25 m. Source: Gillham et al. (1984).

function of vertical elevation z. Thus, the two-dimensional transport equation, including longitudinal as well as transverse dispersion, is given by

$$\frac{\partial c}{\partial t} + u(z) \frac{\partial c}{\partial x} = D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial z^2} \tag{8}$$

The dispersion coefficients D_L and D_T in equation (8) are assumed to be constant and independent of the spatial variations in the horizontal pore velocity. At a more approximate and therefore simpler level of analysis, the same problem may be treated by means of a one-dimensional transport equation in the form of equation (2).

$$\frac{\partial c}{\partial t} + \overline{V} \frac{\partial c}{\partial x} = \overline{D}_L \frac{\partial^2 c}{\partial x^2} \tag{9}$$

where c, $\overline{V}$ and $\overline{D}_L$ represent concentration, pore velocity, and longitudinal dispersion averaged over the vertical thickness of the aquifer. Marle et al. (1967) raise the question as to whether the one-dimensional Fickian dispersion equation (9) is valid in the heterogeneous stratified aquifer. Their answer was "yes," but only after the displacement had occurred over large distances. They related the global or one-dimensional dispersion coefficient $\overline{D}_L$ to the spatial velocity (or hydraulic conductivity) distribution and to the local microscopic dispersion coefficients D_L and D_T.

Equations (8) and (9) illustrate the point that the dispersion coefficient $\overline{D}_L$ is no longer a physical property only of the aquifer matrix; rather, it is a curve-fitting coefficient that depends, in addition to the matrix, on the way in which the advective term averages the aquifer flow heterogeneities.

Lallemand-Barres and Peaudecerf (1978) have presented a figure showing the variations of longitudinal dispersivity, a_L, with horizontal distance from the source (see Figure 4.5). As noted above, these field scale dispersivities are many orders of magnitude larger than the grain size values of a_L obtained in laboratory studies using isotropic media. It is clear that dispersivities in the range of 100 m have little inherent physical significance. They are undoubtedly related to the fact that local heterogeneities in hydraulic conductivity are not represented by the advective term in the transport equation. If the flow field were modeled so as to accurately simulate the macroscopic changes in the magnitude and direction of the velocity, it would not be necessary to use inflated values of dispersivity to represent the aquifer mixing processes.

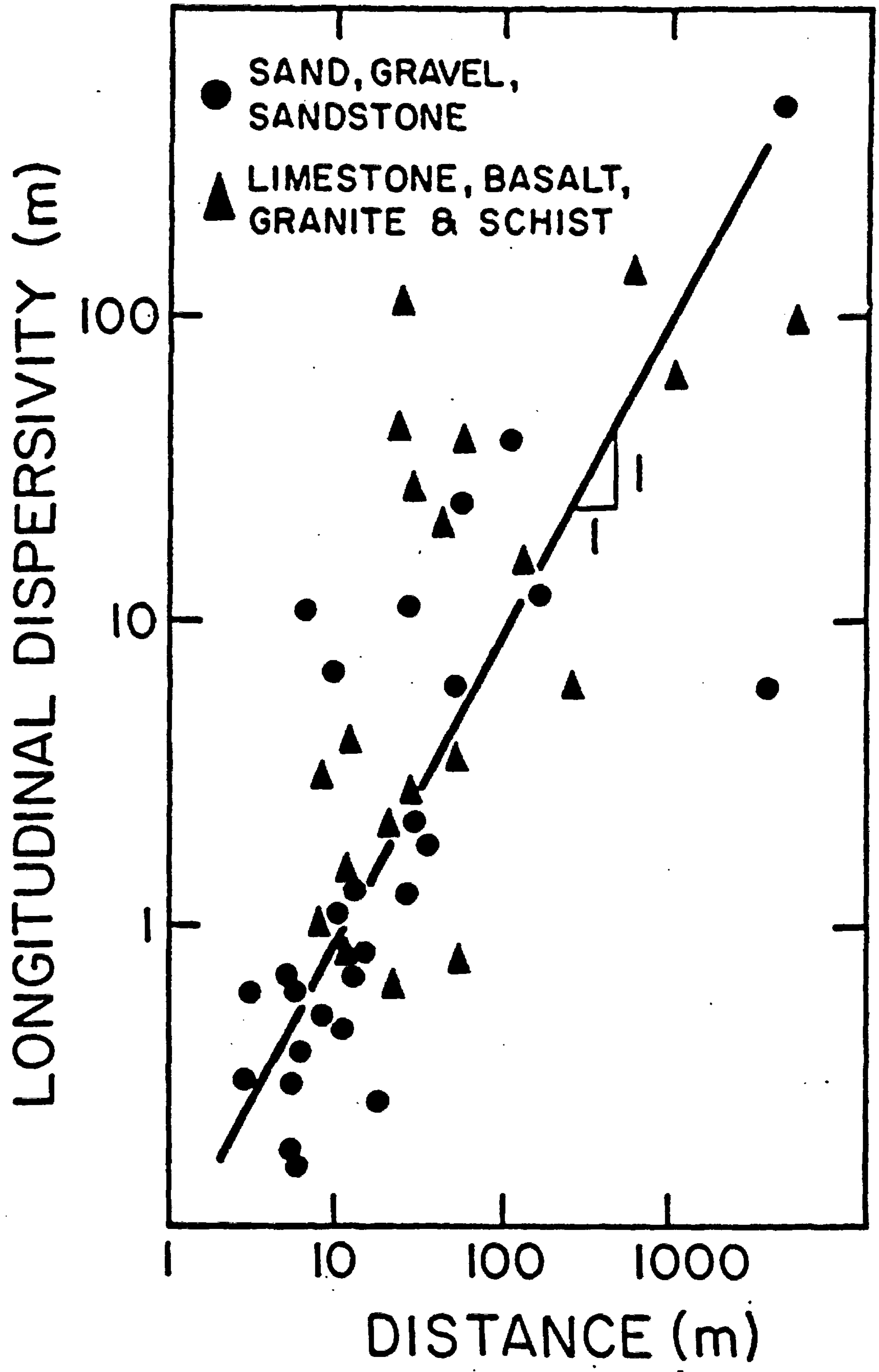

Figure 4.5 Variation of Dispersivity with Distance. Source: Lallemand-Barres and Peaudecerf (1978).

It is concluded that it is possible to generate any number of hypothetical aquifer geometries displaying varying degrees of non-Fickian behavior and dispersivities that increase with distance and time. In most of these deterministic examples, the concentration distribution becomes Fickian at large travel distances and times. The most important question is whether it is possible to have enough field information for a heterogeneous aquifer to define its geometry and corresponding flow properties in sufficient detail to permit application of the type of deterministic models discussed above. In most field applications, the answer is "no." This has led to the development of stochastic hydrology techniques.

4.1.2.2 Stochastic Analysis of Macrodispersion in Heterogeneous Aquifers

Large natural formations always display spatial variabilities of hydrologic parameters such as hydraulic conductivity, transmissivity, and storativity. As a consequence, flow variables such as head, specific discharge, solute concentration, etc., vary irregularly in space. The traditional approach to modeling of flow through heterogeneous formations is deterministic. For example, if the hydraulic conductivity has been measured at a few locations, its distribution in space is specified by a smooth interpolation, and the flow problem is specified by appropriate differential equations. Computer codes are available for solution of general domain geometries and boundary conditions. As Dagan (1982) indicates, this approach is open to criticism for two reasons. First, the geostatistical variables do not vary in a regular manner in space, thus smooth interpolators do not capture their small scale fluctuations; second, synoptic measurements are generally sparse, and the field measurements themselves are subject to uncertainty.

Stochastic hydrology has proceeded in two areas. The first follows the geostatistical approach (Chirlin and Dagan, 1980) of stochastic interpolation which aims at techniques for predicting best estimates and variances of estimation on a spatial grid of variables measured at a few points. The second uses stochastic differential equations. The work of Gelhar (1984) and Gelhar and Axness (1983), which is summarized here, is a good example of this approach. Inherent in the stochastic analysis of macrodispersion is the assumption that the Fickian transport equation is valid at the microscale (as has been well substantiated by laboratory studies). The three-dimensional form, assuming steady state without loss of generality, is given by

$$\frac{\partial}{\partial x_i}(cq_i) = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial c}{\partial x_j}\right) \qquad (10)$$

where q_i is the specific discharge in the x_i direction, in which it is assumed that the microscopic dispersion coefficient D_{ij} is a constant given by the three diagonal terms $a_L q$, $a_T q$, and $a_T q$, where q is the magnitude of the specific discharge vector. In terms of the average velocity V, $V=q/n$, where n is the porosity. It is further assumed that random perturbations about the mean occur in the concentration, specific discharge, and in the logarithm of the hydraulic conductivity. Thus

$$c = \bar{c} + c' \qquad \text{(concentration)}$$

$$f = \bar{f} + f' \qquad \text{(log hydraulic conductivity)} \tag{11}$$

$$q_i = \bar{q}_i + q_i' \qquad \text{(specific discharge)} \qquad i = 1, 2, 3$$

where the bar indicates the means and the prime a zero-mean perturbation. Substituting equation (11) into (10) yields

$$\frac{\partial}{\partial x_i} \left[(\bar{q}_i + q_i')(\bar{c} + c') \right] = D_{ij} \frac{\partial^2}{\partial x_i \partial x_j} (\bar{c} + c') \tag{12}$$

Expanding terms and taking the mean of each term produces the mean equation

$$\frac{\partial}{\partial x_i} \bar{q}_i \bar{c} = D_{ij} \frac{\partial^2 \bar{c}}{\partial x_i \partial x_j} - \frac{\partial}{\partial x_i} \overline{q_i' c'} \tag{13}$$

The second term on the right reflects the macrodispersive flux due to random variations in c and q, whereas the first term on the right represents the microdispersive flux. Subtracting the mean equation (13) from (12) and neglecting second-order terms produces

$$q_i' \frac{\partial \bar{c}}{\partial x_i} + \bar{q}_i \frac{\partial c'}{\partial x_i} = a_{ij} \, q \frac{\partial^2 c'}{\partial x_i \partial x_j} \tag{14}$$

Equation (14) is the stochastic differential equation describing the concentration perturbation c' produced by specific discharge perturbations q'. The specific discharge perturbations are related to stochastic variations in the hydraulic conductivity. Equation (14) is solved by assuming Fourier representations for the random perturbed quantities c' and q'. A general expression for the macrodispersive coefficient A_{ij} defined by

$$\overline{q_i' c'} = - q \, A_{ij} \frac{\partial \bar{c}}{\partial x_j} \tag{15}$$

is developed. In order to evaluate the dispersivity tensor A_{ij}, it is necessary to relate the spectrum of the local flow variation to that of the local log hydraulic conductivity perturbations. This relationship depends on the covariance function used to describe the heterogeneity of the hydraulic conductivity. Thus, the primary macrodispersion coefficient depends on the flow properties and not on the microscopic dispersivities.

Gelhar and Axness (1983) present results of the stochastic analysis in which the statistical properties (variance and spatial correlation length) of actual aquifers are estimated. An example, shown in Figure 4.6, shows spatial variations of log permeability and porosity from a borehole in the Mt. Simon sandstone aquifer in Illinois. The permeability, which varies over four orders of magnitude, illustrates the difficulty of using a deterministic model for this stratified aquifer.

The stochastic analysis gives the following ways of estimating the effective or macroscopic dispersivity tensor A_{ij} in statistically isotropic media

$$A_{11} = \sigma_f^2 \lambda / \gamma^2 \qquad \gamma = q/K_\ell J_1 = \exp(\sigma_f^2/6)$$

where J_1 = the mean hydraulic gradient in the axis of flow;
λ = correlation scale;
σ_f^2 = variance of ln K, the hydraulic conductivity

$$A_{22} = A_{33} = \frac{\sigma_f^2 a_L}{8\gamma^2} \left(1 + 3\,\frac{a_T}{a_L}\right), \qquad A_{ij} = 0, \forall\, i \neq j$$

Once again, we see that the dispersion process is estimated from flow properties.

In summary, it appears that the representation of macrodispersion over large distance and time scales in heterogeneous aquifers by seeking "constant" or "effective" values of dispersivity (as in Figure 4.5) is highly questionable. The solution does not appear to be in undertaking short-term and near-field tracer studies since it is likely that the distances traveled in any reasonable field experiment will be small compared with the scale of aquifer heterogeneities. The most effective approach is to concentrate on the best definition of the flow field through measurement of the aquifer flow properties such as hydraulic conductivity. The choice of a deterministic or stochastic model of the flow field (and the corresponding solute concentration field) is then made on the basis of regularity or irregularity of the flow property.

A different approach to stochastic modeling of dispersive processes in heterogeneous media is represented by the work of Smith and Schwartz (1980) and Simmons (1982). They simulated the solute particle transport in an array of varying hydraulic conductivity blocks having spatial correlations. A line of tracer particles were released at the source side of the region. For each time step, there is a deterministic motion in the direction of the prescribed flow vector and, in addition, there are random displacements parallel and normal to the flow vector. The random displacements are functions of specified longitudinal and transverse microscopic dispersivities and a random number generator. The results produced after many Monte Carlo realizations are similar to the stochastic analysis results discussed previously. Namely,

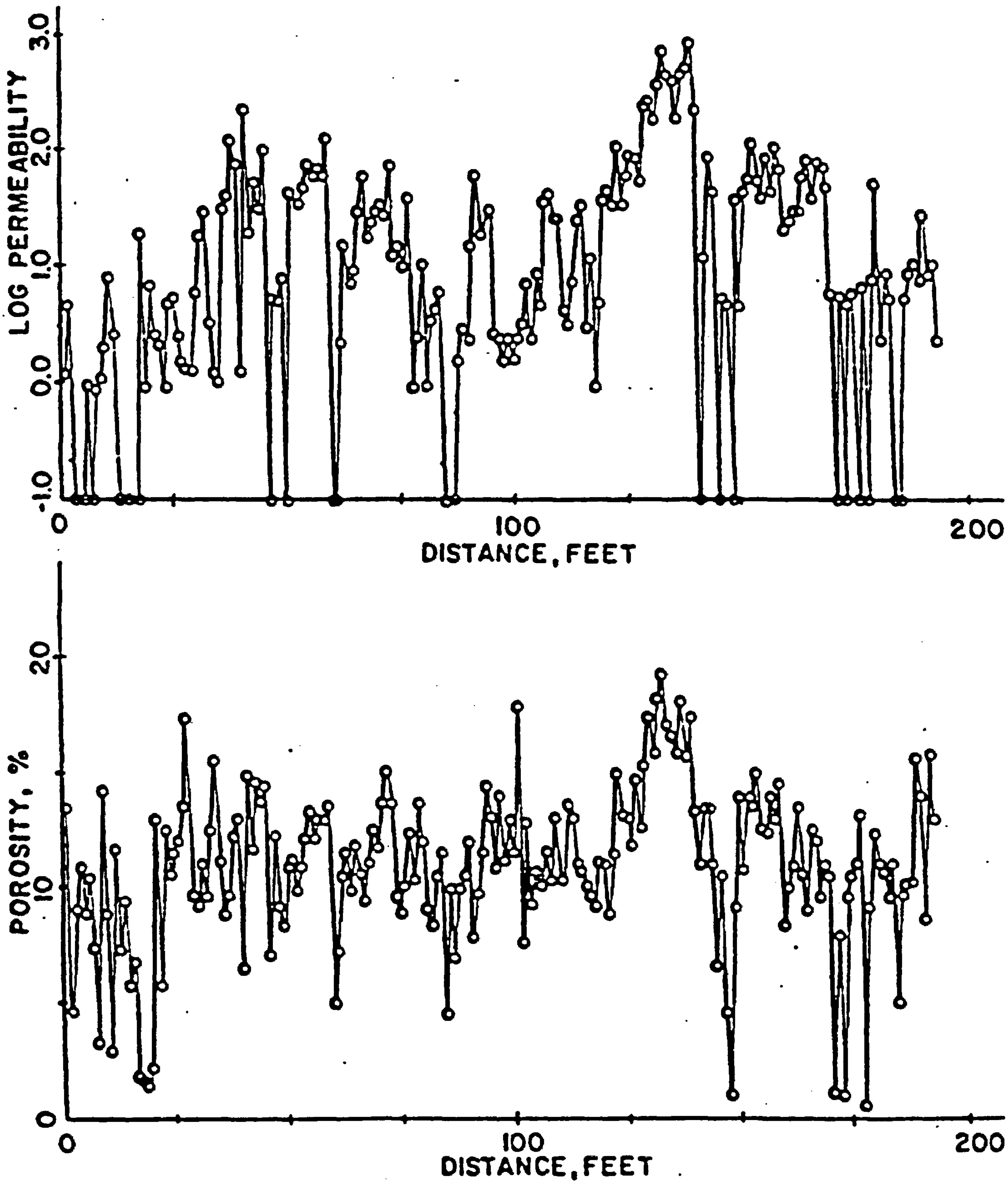

Figure 4.6 Permeability (millidarcy) and Porosity from Laboratory Analysis of Cores from a Borehole in the Mt. Simon Sandstone Aquifer in Illinois. Source: Bakr (1976).

transport behavior could range between Fickian and non-Fickian dispersion depending on the choice of parameters. The random particle displacement approach appears to be concentrated on one-dimensional flow situations probably because of the large amount of computer time required for the Monte Carlo simulations. From this standpoint, the previous multi-dimensional stochastic hydrology approach of Gelhar and his co-workers seems preferable for heterogeneous media.

Smith and Schwartz (1984) have extended the random particle displacement simulation technique to investigate macroscopic dispersion in fractured media. The model is based on the repetitive generation of realizations of a fracture network from probability distributions, describing the fracture geometry, and on a solution for mass transport within each network, using a particle-tracking technique. The approach is limited to two-dimensional, orthogonal fracture sets. The question of Fickian/non-Fickian behavior is investigated, and again the result depends on parameter choice.

4.1.3 Dispersion in Partially Saturated Porous Media

Laboratory studies on dispersion in partially saturated flow in homogeneous, isotropic porous media have been summarized by DeSmedt and Wierenga (1984). In unsaturated systems, variations in the hydraulic gradient and pore velocity are brought about by varying the volumetric water content. It is therefore difficult to study the effect of pore velocity on dispersion at a constant water content because high pore velocities exist only for steep hydraulic gradients, and steep gradients exist only over short distances.

Two approaches have been followed in analyzing longitudinal dispersion in column tests. The first and more traditional approach is to introduce the volumetric water content, θ (cm^3/cm^3), into the transport equation. For example, in the one-dimensional form, equation 9 becomes for a conservative substance

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial}{\partial x}(qc) = \frac{\partial}{\partial x}\left(D_L \theta \frac{\partial c}{\partial x}\right) \tag{16}$$

where q is the water flux per unit area ($cm^3\ cm^{-2}\ sec^{-1}$) and

$$c = \frac{\text{mass of solute/volume of solution}}{\text{total mass of solution/volume of solution}}$$

The breakthrough curves of the unsaturated column experiments showed early breakthrough and tailing. These could be described by the classical Fickian transport equation (i.e., equation 16); however, longitudinal dispersion coefficients 10 to 20 times larger than the saturated case at equal pore water velocities were required. A linear relationship between the longitudinal dispersion coefficient and the pore water velocity $v = q/\theta$ was found as shown in Figure 4.7.

The second approach which provides a better description of the column breakthrough curves is obtained with a model accounting for mobile and immobile water fractions within the partially saturated porous media (van Genuchten and Wierenga, 1976). The transport equation for the mobile fraction is

$$\frac{\partial(\theta_m c_m)}{\partial t} + \frac{\partial}{\partial x}(q\ c_m) = \frac{\partial}{\partial x}\left(D_{Lm}\ \theta_m \frac{\partial c_m}{\partial x}\right) - \alpha\theta_m\ (c_m - c_{im}) \qquad (17)$$

In addition, an equation accounting for the exchange of mass between the two fractions is

$$\frac{\partial(\theta_{im} c_{im})}{\partial t} = \alpha\ \theta_m\ (c_m - c_{im}) \qquad (18)$$

where the subscripts m and im refer to mobile and immobile fraction ($\theta_m + \theta_{im} = \theta$) and α is an interfraction mass transfer coefficient. The advantage of this model is that longitudinal dispersion coefficients obtained from saturated experiments can be used directly. Logically, there should be no essential difference between the saturated and unsaturated dispersive mechanism once the immobile water fraction has been accounted for. Approximately linear relationships between θ_m and θ as well as α and the mobile water pore velocity $v_m = q/\theta_m$ were found as shown in Figures 4.8 and 4.9.

The modeling of flow and dispersive mass transport in the unsaturated zone of heterogeneous soils of the type encountered in the field is not well developed. Yeh and Gelhar (1983) conclude that the unsaturated hydraulic conductivity antistrophy is dependent on the moisture content. Thus, the classical approach to predict flow in heterogeneous media may have to be re-examined. The modeling problem is complicated by dimensionality (three-dimensional flow being common) and spatial variability of soil properties.

Under unsaturated conditions, it is reasonable to expect that dispersivities will increase as the scale of the experiment increases as was observed in the case of saturated flow. Unfortunately, very few field-scale dispersivities have been reported for unsaturated systems. The field observations of Routson et al. (1979) point to the importance of lateral spreading. The dependence of lateral movement on moisture content suggests a soil moisture dependence of the antistrophy of hydraulic conductivity as predicted by Yeh and Gelhar (1983).

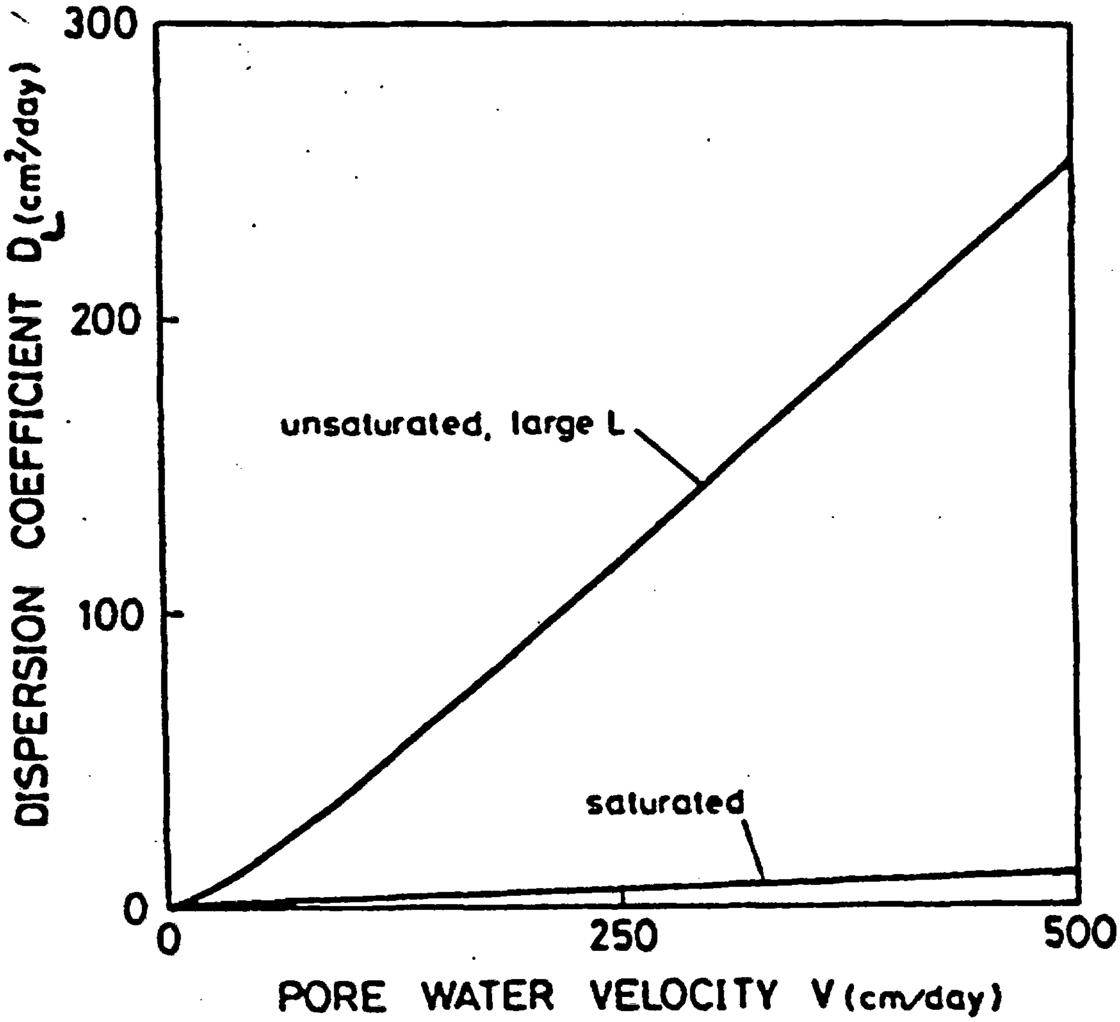

Figure 4.7 Calculated Relations Between Hydrodynamic Dispersion Coefficient and Pore Water Velocity for Long Saturated and Unsaturated Columns.

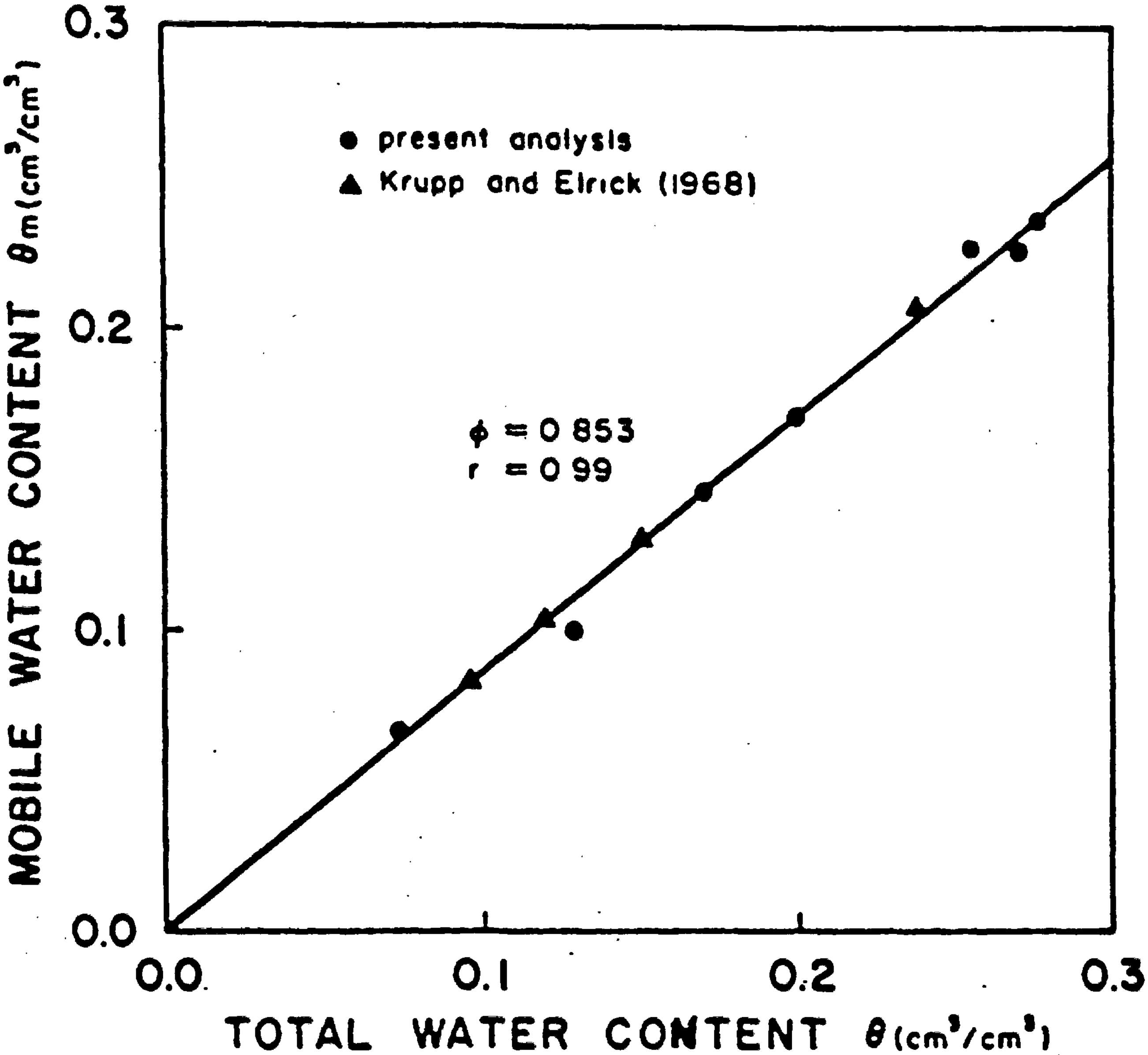

Figure 4.8 Relation Between Mobile Water Content and Total Water Content in Partially Saturated Media.

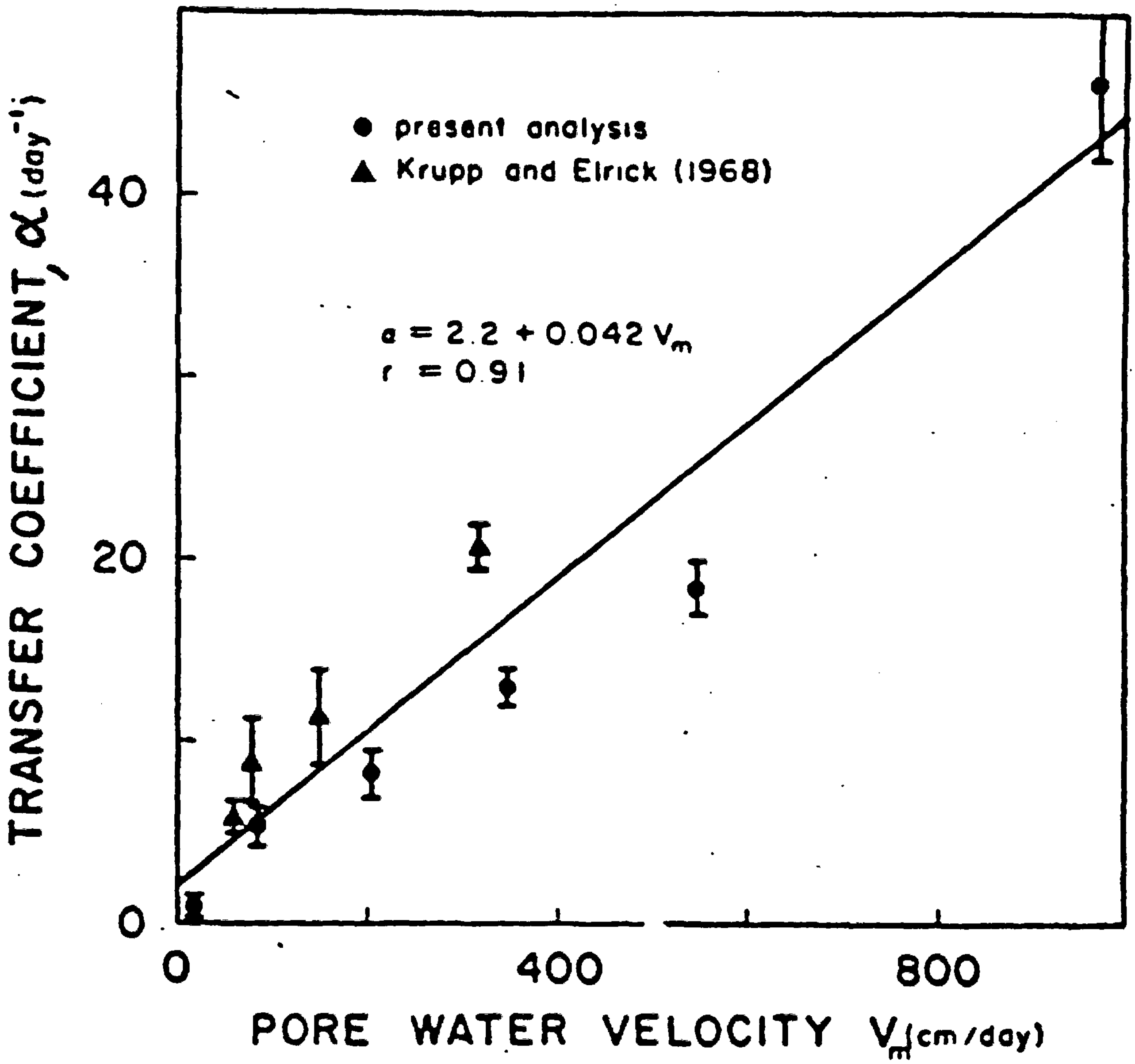

Figure 4.9 Relation Between Transfer Coefficient and Mobile Pore Water Velocity in Partially Saturated Media.

A stochastic approach for the analysis of spatial variability in steady unsaturated flow has been described by Yeh and Gelhar (1983). The corresponding solute transport stochastic analysis problem is in its infancy. The most recent work is by Mantoglou (1984) who considers a modeling framework for treating large-scale unsaturated flow and transport systems. His stochastic approach assumes that local soil properties are realizations of three-dimensional random fields. The local governing flow and transport equations are averaged over the ensemble of realizations of the underlying soil property random fields.

A review of numerical flow and transport models in the unsaturated zone has been prepared by Oster (1982).

4.2 Environmental Pathways and Dosimetry Modeling

The Performance Assessment National Review Group recommends that DOE's long-term performance assessments for geologic waste disposal include the capability of estimating individual doses from releases of radioactivity to the biosphere. Although current EPA and NRC regulations for postclosure repository performance do not require dose calculations, it is reasonable to expect that other parties will request that such calculations be made. Furthermore, estimates of individual dose provide a measure of long-term repository performance that is more closely associated with the fundamental goal of protecting public health and safety than are the performance requirements in the EPA and NRC regulations.

The following remarks are of two types. First, we present a few general comments on environmental transport and dosimetry modeling as it relates to long-term performance assessments for geologic waste disposal. The second set of comments relates specifically to the PABLM code (Napier, Kennedy, and Soldat, 1980; INTERA, 1983a), which is the code that all three DOE Projects currently plan to use for performing individual dose calculations.

4.2.1 General Comments

(1) Any methodology for estimating dose to individuals requires as input release rates and concentrations of radioactivity in the biosphere. Therefore, the models that are used to predict radionuclide transport from a repository to the biosphere must include the capability of calculating radionuclide fluxes and concentrations in order to provide the proper input for the environmental pathways and dosimetry models. Furthermore, the models for transport in the geosphere may need to consider distances of travel to the discharge point in the biosphere that are much longer than the 10-km distance to the accessible environment in the EPA standard.

(2) In estimating individual doses, one is calculating doses to so-called critical groups in the exposed population. The critical group basically consists of those individuals who potentially experience the greatest risks from exposure to the released radioactivity. For some types of releases to the biosphere (e.g., via a small well drilled into a contaminated aquifer), the critical group may comprise only a very few

individuals. For other cases (e.g., releases to a river or to large wells that are used as a source of water for a metropolitan area), the critical group may contain many individuals. The DOE Projects may need to exercise considerable care and judgment in developing exposure scenarios for critical groups, particularly for the tuff and salt sites. The problem for the tuff site is defining exposure scenarios when there is no release to a river and the repository is located in an arid, sparsely populated region. For salt sites, the problem is defining reasonable exposure scenarios when the radionuclides are initially in brine solutions. Another aspect of developing exposure scenarios that requires some care involves defining dietary and other living habits for the critical groups. For example, many analyses make the conservative assumptions that all drinking water comes from contaminated wells or rivers and that all foodstuffs are grown on land irrigated with contaminated water, etc. More realistic assessments of fractional usages of contaminated water and foods are encouraged. A reasonable approach is that of the Canadian methodology in which probability distributions of dietary habits and living patterns are assumed (Lyon, 1981 and 1982). In addition, dose calculations might also need to take into account that living habits thousands of years from now may be quite different than at present. The Canadian program has also developed models to address this problem (Zach, 1982a, 1982b, 1982c; Zach and Sherman, 1984).

4.2.2 Comments on the PABLM Code

This section presents some specific comments on the use of the PABLM code (Napier, Kennedy, and Soldat, 1980; INTERA, 1983a) to estimate long-term individual doses from geologic waste disposal. In applying the code to this problem, it should be borne in mind that PABLM was originally written for routine or accidental releases from nuclear power plants, and that the releases to the biosphere from nuclear waste disposal may be of long duration and will consist of long-lived radionuclides. Our comments are as follows:

(1) Probably the most important deficiency in the PABLM code involves the dosimetric data base for estimating internal dose per unit activity of an inhaled or ingested radionuclide. For geologic waste disposal, most exposures will be via ingestion. The dosimetric data in the code are based on outdated models presented in Publication 2 of the International Commission on Radiological Protection (ICRP) (ICRP, 1959) that should be replaced by models such as those presented in ICRP Publications 26 and 30 (ICRP, 1977 and 1979). It is not a trivial matter, however, to choose a proper dosimetric data set based on current ICRP methods. Internal dosimetry codes developed by different Federal agencies contain significant differences, particularly with regard to assumptions used in the models for calculating doses to the lung and to the skeleton and soft tissues in bone. It is mainly for this reason that differences in calculated effective dose equivalents (ICRP, 1977) of a factor of two between codes are not uncommon for some radionuclides, and even greater differences can be found for specific body organs. In addition, the calculations in ICRP 30 (1979) and most other codes assume parameters that are appropriate for exposures in the workplace but may be inappropriate for environmental exposures. An important example of

this is the value of the GI-tract uptake fraction for environmental exposures to plutonium and neptunium. The ingestion dose to all organs except the GI-tract is directly proportional to this parameter. For occupational exposures, the ICRP currently recommends uptake fractions of 10^{-4} for plutonium and 10^{-2} for neptunium, and these values are used in most current dosimetry codes. For environmental exposures, however, there is considerable evidence that the best value of the uptake fraction is 10^{-3} for both elements(Thompson, 1982a, 1982b; Kocher and Ryan, 1983); i.e., ingestion doses per unit intake should be increased by a factor of 10 for plutonium and decreased by a factor of 10 for neptunium compared with standard ICRP 30 results. The point of this discussion is that it would be inappropriate for the DOE to simply adopt dosimetric data from ICRP 30 or from codes such as INREM-II (Killough et al., 1978; Dunning et al., 1981) or RADRISK (Dunning and Eckerman, 1984) without exercising scientific judgment in the choice of models and input parameters that would be appropriate for environmental exposures to important radionuclides in high-level waste.

(2) The PABLM code neglects inhalation of resuspended radionuclides from surface soils. This exposure pathway is likely to be relatively unimportant for most radionuclides in high-level waste, but resuspension could be important for plutonium and americium if a substantial fraction of the release to the biosphere is assumed to be deposited on the land surface (e.g., via irrigation from a contaminated aquifer or river). The importance of resuspension for these nuclides and this exposure scenario arises from the low bioaccumulation in terrestrial food chains coupled with high lung doses per unit activity inhaled. Some care and judgment must be exercised in choosing a resuspension model for long-lived radionuclides that are deposited on the ground surface over long periods of time. This is because the availability of a radionuclide for resuspension decreases with time as the activity penetrates below the surface. For some reasonable approaches, see Bennett (1976).

(3) The PABLM code does not consider removal of activity from the soil root zone over time via downward migration. This affects the important dose rates from terrestrial food chains, and the code does not consider reductions in external ground-surface exposure over time due to the penetration of deposited activity into soil. At present, the time dependence of dose rates from terrestrial food chains and ground-surface exposure for a given initial deposition are determined only by the radiological decay constant. For long-lived radionuclides, however, mechanisms other than radioactive decay, e.g., infiltration into the ground via percolating rainwater, can be more effective than radioactive decay in determining dose rates over long time periods. Thus, these mechanisms can lead to significant reductions in estimated dose rates for these exposure pathways. The recent report of the EPA's Science Advisory Board Subcommittee on high-level waste disposal (USEPA, 1984b) contains descriptions of models that would be adequate for estimating dose rates over time for terrestrial food chains and external ground-surface exposure.

(4) The models used in PABLM for estimating dose rates from terrestrial and aquatic food chains per unit concentration of a radionuclide in soil or surface waters are generally adequate for application to geologic waste disposal. We recommend, however, that the data base for the various bioaccumulation factors be examined and updated as necessary to reflect currently accepted values. Recent publications from Yook Ng at Livermore are probably the best sources of these data (Ng et al., 1978; Ng, 1982a, 1982b; Ng et al., 1982).

(5) For a release of radioactivity to a surface water system, the PABLM code calculates radionuclide concentrations in the water from the radionuclide release rate, the flow rate in the water body, and a so-called mixing parameter which takes into account that the release is generally not from a point source. The code considers removal of radioactivity from the water column via sedimentation only for the purpose of estimating concentrations in shoreline sediments and resulting external radiation doses, but does not consider the reduction in water concentration itself due to sedimentation. We recommend that the model for estimating radioactivity concentrations in surface waters be modified to include the effects of sedimentation on reducing these concentrations and, thus, on reducing doses by aquatic pathways. A suitable model was developed by Booth (1975) and has been implemented by the U.S. Nuclear Regulatory Commission (1978). The Booth model is a linear compartment model that includes compartments for receiving waters, exchangeable sediments (i.e., a compartment from which deposited activity can be returned to the water column), and buried sediments. Calculations with this model by Kocher et al. (1980) have shown significant reductions in surface-water concentrations due to sedimentation for strongly sorbed, long-lived radionuclides such as plutonium.

(6) For a release of carbon-14 to surface waters, the PABLM code assumes that the specific activity of carbon (i.e., pCi of carbon-14 per kg of total carbon) in the biosphere is the same as the specific activity in the surface waters. For a release to surface waters, this assumption probably provides a gross overestimate of carbon-14 in the biosphere and, thus, in human intakes. Although definitive studies of the origin of carbon in terrestrial biota have not yet been performed, it is most likely that photosynthesis of atmospheric carbon is by far the most important pathway for human intakes of carbon. For a release to surface waters, the specific activity of atmospheric carbon will be much less than the specific activity of carbon in the water. The Projects should consult with experts in environmental cycling of carbon to determining suitable modifications of the present model that would result in more realistic dose estimates for carbon-14 released to surface waters.

In conclusion, some modifications of the environmental pathways models and the dosimetric data bases would appear to be in order in applying the PABLM code to the estimation of individual doses from high-level waste disposal. These modifications will require the application of expert judgment to ensure that they are appropriate to the problem at hand. Some modifications, such as the choice of a dosimetric data base, probably can be applied uniformly to all repository sites. Other modeling needs, such as the definition of critical groups and exposure scenarios, will be more site specific.

4.3 Geochemistry

The PANRG considers the use of geochemical information an integral part of performance assessment and specifically requested briefings on the Projects' approaches to radionuclide migration retardation by geochemical processes such as adsorption and precipitation. The Projects did not respond adequately to our request. The following comments relate to the importance of geochemical processes.

An understanding of ground water/rock geochemistry is not only essential to predict radionuclide mobilities in the event of a breached repository, but also provides unique information regarding the degree of isolation that may be provided by the host rock as indicated by the age of the ground water. Neither of these points appeared to be properly emphasized in the presentations of the three Projects. As to the latter, natural radionuclides such as tritium, carbon-14, chlorine-36, and radiogenic isotopes of helium, neon, and argon can be used to estimate the mean subsurface residence time of ground waters, whether a few years or a few thousand years or more (Andrews and Lee, 1979; Bentley et al., 1984; Davis and Bentley, 1982 and Zaikowski et al., 1983). Recent studies of natural radioisotopes of thorium, uranium, and radium in fresh and saline ground waters address the determination of both rates of adsorption and of the extent of adsorption of the radioisotopes (Krishnaswami et al., 1982). Although such information would shed light on the probable behavior of thorium, uranium, and radium that might leave a breached repository, limitations on the applicability of the methodology have been noted (Rama and Moore, 1984).

There is an extended discussion of the role of natural radionuclides as a validation aid in Technical Observation No. 7.

The origin of the ground water can be further identified through stable isotope analyses of, for example, the actinides, oxygen, chlorine, hydrogen, carbon, and sulfur. These analyses can give some information concerning the sources of water containing these elements, precipitation temperatures, extent of evaporation of the water, etc. (Fritz and Fontes, 1980). Chemical analyses of the actinide elements may reveal, for example, that the ground water at a particular location is already saturated with respect to uranium, making the leaching of uranium from spent fuel unlikely.

Geochemistry is also important as an input to the predictions of repository performance. Geochemical processes such as adsorption, precipitation, colloid formation and matrix penetration can significantly affect radionuclide transport. To predict whether and how a particular chemical or isotopic species is mobilized, transported and deposited requires 1) understanding of the processes involved; 2) thermodynamic properties of the species and solids involved; and 3) rates of reaction among these species and solids. There is good understanding of many important geochemical processes which affect radionuclide migration and these are now incorporated into mathematical models that may assist in predictive calculations. The geochemical models now available permit at least a semi-quantitative assessment of the roles of adsorption and desorption (e.g., MINEQL; Westall et al., 1976), mineral precipitation and dissolution (e.g., PHREEQE; Parkhurst et al., 1982; and EQ3NR, Wolery, 1983) for elements such as uranium, thorium, and radium and their complexes. Models are also capable of combining complex adsorption and precipitation with transport (Jennings et al:, 1982; Miller and Benson, 1983; Pearson, 1984). Such analyses require an adequate set of thermodynamic state functions, transport coefficients, and reaction rate coefficients for the water/rock system. The most fundamental of these needs is for a sufficiently accurate and complete data set of thermodynamic properties for important radionuclide aqueous species and solids at temperatures from 25 to 250°C. Such a data set is lacking. Apparently, no consensus exists among the Projects as to which thermodynamic data set or sets for the radionuclides should be adopted. Certainly, a single set for radionuclides and related elements in the waste package and the water/rock system should be developed and agreed upon. An effort to compile a set of internally consistent thermodynamic data is underway at the OECD Nuclear Energy Agency involving the U.S. Projects and others. The above recommenation is qualified by observing that a thermodynamic data base should be developed for <u>important</u> radionuclides only. Various screening transport studies can be and have been performed to identify key radionuclides. Thermodynamic data should be developed for these key radionuclides, <u>not</u> all radionuclides.

Radionuclide adsorption is an important retardation process and it generally depends on 10 or more independent variables. These variables include temperature, solution ionic strength, complexation, electrolyte ion concentrations, competition among elements for adsorption sites, and surface properties of each sorbent mineral, such as surface capacitances, surface area, charge and potential. A computer code called MINEQL (Westall et al., 1976) that can be used to model these adsorption results, and to predict adsorption behavior, has been described in detail by Davis et al.(1978). Some of the empirical constants and parameters needed in adsorption modeling are available for several important dissolved radionuclides and sorbent minerals. These include dissolved lead, uranium, thorium and radium, and the sorbing phases kaolinite, quartz and amorphous silica, ferric and some manganese oxyhydroxides, and several other clays and zeolite minerals (Hsi and Langmuir, 1983 and 1984; Catts and Langmuir, 1983; and Riese and Langmuir, 1983). However, more research is needed before the model can be applied with confidence to the adsorption of transuranic elements, and to adsorption from brines or at elevated temperatures. The Projects should obtain site-specific data in the Site Characterization process for use in adsorption models.

It does not appear reasonable to use distribution and retardation coefficients (K_d and R_d values) measured under laboratory conditions that are vastly different from those likely in a repository without consideration of the various controls (i.e., true adsorption, precipitation and co-precipitation) on retardation. The lack of detailed knowledge about site-specific geochemical conditions, plus the difficulty of incorporating detailed geochemical reactions in transport calculations (Rubin, 1983), make the use of the K_d and R_d approach almost inevitable at present for complex flow regimes. To the extent possible, therefore, the K_d and R_d values used should be functions of variations in controlling processes rather than single numbers. In the tuff project, for example, sorption or retardation studies are planned using crushed Yucca Mountain tuff. The effects of CO_2 pressure, microbes, and drilling additives on values of K_d and R_d will be considered. For elements such as strontium, barium, europium, cerium and americium, K_d and R_d values have been shown to vary typically by two or more orders of magnitude in single drill holes in the tuff. These variances occur for reasons which need to be evaluated. Using a model which has K_d as a single independent variable would not yield results in which a high degree of confidence can be placed. The Projects should be careful when using such a simplified approach, and the reasons for using such an approach should be documented, as suggested in General Observation No. 7.

4.4 Some Water Saturation Measurement Techniques in Unsaturated Tuff

Performance assessments in partially water-saturated tuff require not only an accurate measurement of the in-place water saturation and its variation with height above the water table, but also an evaluation and prediction of the water flow capacity of the rock at various saturations.

Reports made to PANRG by LLNL and SNL personnel revealed that they have not, to date, been successful in using electric/radioactive logs run in wells, nor the analysis of recovered cores, to define the tuff water saturation. A problem of a similar nature was encountered by the oil and gas industry in the early 1970s by those companies attempting to find and develop gas reserves in very low permeability (microdarcy) formations. After several years of study, workable procedures were developed for logging and coring wells to provide reliable information on the in-place water saturations of such formations.

In general, it was found that the invasion of drilling fluid filtrate (water) into the periphery of the well bore, which can severely complicate the interpretation of logs to obtain formation water saturations, could be significantly reduced, or even eliminated, by maintaining the bottom hole pressure (at the drill bit) during coring to be equal to or less than the formation pressure. Similarly, the invasion of mud filtrate water can be eliminated if an oil-based drilling fluid is used, in which case the filtrate entering the formation would be oil. Again, controlled pressure conditions should be used so as to minimize the possible entry of oil into the formation immediately adjacent the bore hole. Service firms, such as Schlumberger Well Surveying Corporation, were very helpful to the industry in working with selected oil companies like Amoco and Champlin to develop effective and reliable log interpretation procedures for low permeability horizons. These procedures take advantage of both shallow investigating devices (for the zone invaded by mud filtrate) and deeper investigating devices for the non-invaded zone. When run together, these two types of logs will permit a more reliable interpretation of the true formation saturation. A suite of porosity measuring logs is also used to not only define formation porosity, but also can provide a measure of original gas saturation if mud filtrate invasion depths are shallow (inches). The results of some of this work have been reported at the annual Tight Gas Symposium held in Denver each spring, sponsored by the Society of Petroleum Engineers which publishes proceedings of these meetings.

With regard to obtaining reliable field measurements of water saturation values through the analysis of cores, the processes discussed above (i.e., coring with a water-based drilling mud under "balanced" pressure conditions or use of an oil filtrate mud) have proved to be successful. The latter process, (i.e., coring with an oil filtrate fluid) has been widely used within the petroleum industry since the early 1950s to obtain cores that retain the reservoir "in-place" water saturations to a depth of several thousand feet. This process has been documented frequently in the petroleum literature. In the development of these processes, the industry also attempted "dry" coring (i.e., the circulation of only small amounts of air or gas during coring) on numerous occasions. This process was consistently found to heat the drilled cores to the extent that some of the in-place water was evaporated, thus causing measured core water saturations to be lower than the original values in the reservoir.

Almost all of the major drilling fluid companies have developed oil-based drilling fluids that are suitable for coring. These drilling fluids normally contain surface active agents (needed to stabilize the mud) that may alter some of the properties of invaded cores. This potential contamination should be considered when the cores are to be used for other types of laboratory tests in which the surface activity of the rock surfaces is an important parameter. However, the core water saturations should remain unchanged unless the water saturation is mobile. The low level of water mobility in the partially saturated tuff should make this formation suitable for coring with an oil-based fluid. However, if the oil contamination of the formation surrounding the well is considered to be a deterrent to later well tests, it may be necessary to drill a sacrificial well with oil just to obtain the needed water saturation information.

CHAPTER 5

SUMMARY OF OBSERVATIONS AND RECOMMENDATIONS

5.1 General Observations

The general observations of the PANRG relate to the management and institutional aspects of the performance assessment activities. They address the following three areas:

(1) resources (both human and budgetary)
(2) program planning, coordination, and management
(3) communications (intra and inter-project, project-Headquarters, and inter-agency levels)

5.1.1 Resources

Based on the interactions between PANRG and the project staffs during the briefing sessions conducted and the direct working contacts with the Projects by some members of the PANRG, it was concluded that a resource of competent professional scientists and engineers is available to carry out the performance assessment work that will be required. The experience level, which appeared to be somewhat uneven and lacking in some instances, will obviously improve as the work progresses. There were indications that the budgetary resources allocated to performance assessment needs are inadequate. This may also apply to manpower levels as well.

5.1.2 Program Management

Although there was indication of recent efforts to address the issue of more coherent management of the overall performance assessment program (e.g., the establishment of a Performance Assessment Coordinating Group organized by the OCRWM-HQ), the need for more coherent program management was evident from several standpoints. For example, currently there was little indication of consistent planning in this area. Areas of common concern among the Projects were not being addressed on a coordinated basis. Identification of issues related to the licensing, processes, and approaches to their resolution did not appear to be addressed in a systematic way, and guidance and direction from HQ appeared to have been minimal.

5.1.3 Communications

Working communications at all levels appear to need improvement. Such improved communication would be of major benefit to the overall program. Within the Projects, model developers need to communicate and work closely with laboratory and field people. Better communication among the performance assessment staffs of the Projects can promote more effective solutions to common problems. More effective working relationships and communications with EPA and NRC are essential to a successful licensing process.

5.2 General Recommendations

The recommendations of the PANRG associated with the general observations summarized above are implicit in those observations. They include, as perhaps a central feature, the development of a coordinated and integrated Performance Assessment Plan. Such a plan would address, among other things, the specific issues requiring performance assessment application in the areas noted in Section 1.1, and human and budgetary resource requirements, communication, and coordination mechanisms at all levels, particularly at the OCRWM-NRC level. Such a plan would also provide a major tool for program management and timely and effective program implementation.

Because performance assessment is essentially based on the exercise of professional judgment, clear and supported documentation of all of those judgments should be an integral part of all performance assessment work.

It was also recommended that a continuing, independent performance assessment review mechanism be established.

5.3 Technical Observations and Recommendations

The PANRG's technical observations covered the broad range of scientific and technical disciplines inherent in the performance assessment of a geologic repository. One perspective of these observations is in terms of the performance objectives for the repository contained in the proposed EPA standard (1982) and the NRC regulations (1981); namely, containment, radionuclide release rate, ground-water travel time to the accessible environment, and cumulative radionuclide release to the accessible environment. Although radiological impacts are not explicitly included in the regulatory performance objectives, it is desirable to evaluate such impacts (i.e., calculation of doses) of potential releases. Considerations of the phenomenology of corrosion, waste form dissolution, geochemical reactions, and flow and transport are obviously intimately involved in the modeling and analysis of the repository system and its components. These phenomenological considerations, the models used to describe and characterize them, and the methodologies used to address the system and component performance are overlain by important analytical considerations. Issues such as the time extrapolation of short-term laboratory and field data, the handling of uncertainty and variability of data, and the probabilistic nature of many of the factors relating to repository behavior and the assurance of model adequacy and validity represent important aspects of performance assessment. Further, there is the important question of determining what constitutes an adequate scientific understanding or basis for rational technical, or engineering decisions necessary for component and system design, construction and operation.

The PANRG's technical observations and associated recommendations reflect, with varying degrees of specificity, all of the factors noted above. In this connection, it must be recognized that, in the absence of site-specific data (particularly geochemical data) and the inadequate data bases for such phenomena as container corrosion and spent fuel dissolution, there is of necessity a paucity of performance assessment results.

In general, from a technical standpoint, the current situation in performance assessment can perhaps be summarized as follows:

- Much of the necessary site-specific and component-specific data are not yet available, but many of the necessary experiments and tests to acquire such data have been defined and can be carried out.
- Models may well require some refinement or modification based on the data to be acquired. Assurance of model adequacy is largely dependent on in-situ or site-specific tests or investigations yet to be carried out but whose scope and nature are identifiable.
- Techniques and methodologies for handling uncertainties in data and performance sensitivities to specific factors appear reasonably well developed but few results are available and therefore their usefulness and validity cannot be evaluated.
- The Projects' work to date in performance assessment does not reflect sufficient technical evaluation by the Projects themselves of the adequacy of predictive techniques, of the relevance and adequacy of experiments and tests to verify and validate those predictive techniques, and of the adequacy of input data for making such predictions.
- The probabilistic aspect of several facets of performance assessment has yet to be incorporated appropriately into the models and assessment methodologies.
- Sound, acceptable bases for time extrapolation of phenomenological data (e.g., corrosion and dissolution) have yet to be developed.

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Appendix A

Charter for the Performance Assessment National Review Group

Introduction

The Waste Isolation System Panel (WISP) of the National Research Council/ National Academy of Sciences (1983) had several important observations related to performance assessment within the National Waste Terminal Storage (NWTS) program, now under the Office of Civilian Radioactive Waste Management (OCRWM). First, the panel observed that the selection and the licensibility of sites for geologic repositories for disposal of high-level wastes will depend heavily on the predicted performance of the waste isolation system. Second, the panel observed that insufficient resources have been devoted to the performance assessment of the waste isolation system.

For the purpose of this group, performance assessment can be defined as the development, testing and application of one or more mathematical models which trace the inventory, decay, potential movement and reactions of radionuclides emplaced in a geologic repository back to the biosphere, including calculations of the resultant effects on people.

In particular, the panel recommended that overall technical review should be done on geologic disposal. This technical review should be done with emphasis on relating program efforts to the goal of developing a repository with predictable satisfactory performance. The charter and expertise of review groups should be broad enough to ensure adequate consideration of interdisciplinary problems, and it should develop a greater systems analysis content in its management and review.

The panel also recommended that a review should be made of the techniques for calculating radiation doses that could result from water contaminated by a geologic repository, and the uncertainties in these calculations should be determined. Consideration should be given to the development of standardized methods for calculating these radiation doses, including the development of appropriate and updated metabolic parameters and environmental transfer parameters for the important radionuclides. These techniques for dose calculation and the parameters used in them should be reassessed periodically.

In response to these observations, Weston is establishing a group of nationally-recognized experts who will be used to assist Weston in a national review of performance assessment activities in the OCRWM. The purpose of establishing the review group is to recommend, as appropriate, specific actions which should be taken in order to improve the performance assessment work by each project and to assure the adequacy of the technical approach for demonstrating compliance with DOE Guidelines on siting, with NRC's 10 CFR 60 and with EPA's 40 CFR 191.

The Performance Assessment National Review Group (PANRG) will specifically review the development, benchmark testing, verification, validation, and application of the mathematical models that are employed to simulate the migration of radionuclides from the waste package, through the geologic host media, and finally to the accessible environment.

This charter for the PANRG discusses the rationale, objectives, scope of work, general approach and schedule for the national review group.

Rationale

The OCRWM projects will have to demonstrate with reasonable assurance that the waste isolation system proposed for their particular site is capable of isolating nuclear waste in compliance with 10 CFR 60 and 40 CFR 191. Because of the long time periods involved and the complexity of the system, this demonstration will be indirect, through mathematical modeling of a large number of interactive processes. There is a need to ensure that the approaches in such complex modeling will provide reasonable assurance of compliance with the regulations, will be technically defensible, and will be adequately documented.

Objectives

The objectives of the PANRG are to: 1) provide an independent review of the performance assessment work currently being sponsored by OCRWM projects, and 2) recommend to Weston and the project offices appropriate improvements in performance assessment which are responsive to the concerns expressed in the National Research Council/National Academy of Sciences report, "A Study of the Isolation System for Geologic Disposal of Radioactive Wastes." In addition, the PANRG is to identify any improvements in performance assessment which may significantly contribute to the demonstration of compliance, technical defense of the modeling, or documentation of the computer codes.

General Approach

Weston will retain under subcontract a number of experts, who are

- without significant conflict of interest,
- knowledgeable in mathematical modeling of radionuclide migration, leaching, and dose to man, and
- knowledgeable in the licensing process.

In addition to these core members of the PANRG, the PANRG may involve, through Weston, advisors for specific topics.

The PANRG will first consider the overall approaches used by each project and any unique site-specific requirements in the performance assessment at given project sites. Subsequent meetings will focus on specific topics, such as ground water flow or quality assurance. Each meeting may therefore differ in the level of detail and participation by advisors to the PANRG. The review is being conducted at the time each project is preparing an overall Performance Assessment plan.

Management

Weston will provide the necessary logistical support and coordination as well as receiving the recommendations of the PANRG.

Dr. Joseph A. Lieberman will chair the PANRG. Dr. William W.-L. Lee of Weston will serve as executive secretary of the Group, as a non-voting member.

Scope of Work

Current plans for the first PANRG meeting call for a general orientation in the DOE-OCRWM program and applicable regulations, e.g., 10 CFR 60 and 40 CFR 191, as well as the overall approaches utilized by each project and any unique site-specific requirements in the performance assessment at given project sites. The second meeting will involve presentations by each project office of their current performance assessment plan and available results. Subsequent meetings will specifically address the following topics:

1. The PANRG shall review current results of the projects performance assessments. Are the predictions sufficiently reliable for licensing purposes? What improvements in performance assessment activities at each project would enhance the basis of a license application. Have uncertainties in the predictions been suitably estimated and evaluated? Are there sufficient plans to demonstrate compliance with the probabilistic EPA standard?

2. How could the overall systems performance work be improved? How should allocation of the safety contribution for the subsystems, i.e., waste package, repository and site, be made relative to overall systems performance?

3. How could the modeling of the subsystems be improved?

4. How could the development and analyses of disruptive scenarios be improved?

5. How could software quality assurance be improved, particularly for documentation, benchmarking, verification and validation?

6. How could the link between data acquisition and modeling be improved?

7. Should subsystem models be standardized across projects?

8. Are there improvements needed in the definition of the role of performance assessment for each project?

9. What additional guidance and/or standardization would be helpful to the DOE and its project offices?

The following are examples of some anticipated results from the PANRG:

a. Judgement regarding the status of work by the Projects. For instance, the PANRG might evaluate the suitability of the approaches taken by projects to handle processes. They might also evaluate the achievability of performance targets within uncertainty bounds.

b. Recommendation on approaches. The PANRG might recommend the suitable approaches to demonstrate compliance with EPA/NRC rules, and suitable methods in uncertainty/sensitivity analysis.

c. Suggest alternate approaches. The PANRG might suggest different treatments of physical processes in the model for greater scientific credibility. The Group might also suggest improved methods of presentation of results.

d. Suggested follow up activities by projects to improve performance assessment.

In addition, the PANRG may identify additional specific topics of review; within the scope of this charter. An agenda for site visits may also be developed, if needed, for the PANRG review.

Schedule

Attachment A is a proposed schedule for the initial meeting of the PANRG, subject to availability of the group members and the appropriate project office personnel.

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Appendix B

Brief Professional Profiles

Performance Assessment National Review Group

Joseph. A. Lieberman is president of OTHA, Inc., a private engineering consulting firm. He received his doctorate in engineering from the Johns Hopkins University. Dr. Lieberman has been involved in high-level radioactive waste management since the early 1950's, and was the first Director of the Office of Radiation Programs at the U.S. Environmental Protection Agency. At OTHA, Inc., Dr. Lieberman consults frequently for the electric utilities on nuclear waste related matters. He is the chairman of the Performance Assessment National Review Group.

Stanley N. Davis is a professor in the Department of Hydrology and Water Resources at the University of Arizona. Dr. Davis is a world renowned authority on ground-water hydrology. He received his doctorate from Yale University and has taught at Stanford University, University of Missouri, Indiana University before joining the University of Arizona. Dr. Davis is the author of Hydrogeology, other text-books and numerous journal articles. He has done consulting in radioactive waste management since the mid-1970's.

Donald R. F. Harleman is a Ford Professor of Engineering at the Massachusetts Institute of Technology. He received his doctorate from M.I.T. and has taught at M.I.T. since 1950. Dr. Harleman has over 30 years of experience in modeling fluid transport of pollutants. He was a pioneer in the modeling of heat discharges from power plants and was an expert witness on the topic many times. Dr. Harleman is a member of the National Academy of Engineering.

Ralph L. Keeney is a professor in the Department of Systems Science at the University of Southern California. Dr. Keeney received a doctorate in operations research from M.I.T. and was on the faculty there for several years. He is an expert in decision and risk analysis. Dr. Keeney has extensive experience in site selection for controversial facilities, such as nuclear power plants; and risk analysis for hazardous facilities, such as liquefied natural gas plants. His most recent book is Siting Energy Facilities and he is a co-author of Acceptable Risk.

David C. Kocher is a research staff member and Group Leader with the Health and Safety Research Division of Oak Ridge National Laboratory. He received his doctorate in physics from the University of Wisconsin. In recent years Dr. Kocher has performed research on uncertainties in performance assessment of potential high-level waste repositories, and on pathways of human exposure to radionuclides dispersed in the environment.

Donald Langmuir is a professor of geochemistry at the Colorado School of Mines. He taught previously at the Pennsylvania State University, and received his doctorate from Harvard University. Dr. Langmuir is an internationally recognized expert in fundamental and applied aspects of ground-water geochemistry. In the last twenty years, he has consulted and lectured extensively. He is the author of well over 100 publications and reports on thermodynamic principles, basic soil and ground-water geochemistry, and applied ground-water geochemistry in mineral exploration and mining and toxic and radioactive waste disposal.

Robert B. Lyon is Acting Director of Canada's nuclear fuel waste disposal program. He holds a master of science in nuclear reactor physics and technology from Birmingham University. His permanent assignment is head of the performance assessment work in the Canadian nuclear fuel waste disposal program. Mr. Lyon is a co-inventor of SLOWPOKE, an operator-free nuclear reactor.

William W. Owens is a private consultant in Tulsa, OK. He holds a master degree in petroleum engineering from the University of Oklahoma. Until his retirement early in 1984, Mr. Owens spent 33 years with AMOCO conducting and directing research on rock properties, multiphase flow in porous media, and reservoir analysis. Mr. Owens has published a number of papers, won a number of patents and in 1978-79 served as a Distinguished Lecturer for the Society of Petroleum Engineers.

Thomas H. Pigford is professor and chairman of the Department of Nuclear Engineering at the University of California, Berkeley (1959-). He received his doctorate in chemical engineering from M.I.T., and was a member of the M.I.T. chemical engineering faculty from 1950 to 1957. From 1963 to 1977, Dr. Pigford served on the Atomic Safety and Licensing Board of the Atomic Energy Commission and Nuclear Regulatory Commission. He is a member of the National Academy of Engineering and a member of the National Research Council's Board on Radioactive Waste Management. He chaired the National Research Council's Waste Isolation System Panel, which issued the report A Study of the Isolation System for Geologic Disposal of Radioactive Wastes (1983). He is a co-author of Nuclear Chemical Engineering and has extensive research publications in nuclear engineering, radionuclide migration, and mass transfer.

William W.-L. Lee is the Executive Secretary of the Performance Assessment National Review Group. He is on the Performance Assessment staff of R. F. Weston, Inc. He received a doctorate in engineering from M.I.T. Prior to joining Weston, he was a faculty member at the University of Pennsylvania.

AGENDA

Performance Assessment National Review Group
First Meeting: Overall Safety Assessment
April 18-20, 1984
Rockville, Maryland

Day 1

9:00 a.m.	Greetings and Introductions	Lee
9:15	Principal DOE Concerns	Cooley
9:45	Relationship of PANRG to WESTON and DOE-HQ	
10:00	Break	
10:15	The Role of Performance Assessment as Specified by the Siting Guidelines	Hanlon
11:00	Compliance with the EPA Standard	EPA
12:00	Lunch	
1:30	The NRC Regulations, Demonstration of Compliance and NRC's Methodologies	NRC
2:30	Questions for EPA & NRC speakers	
3:15	Executive Session	PANRG
5:00	Adjourn	

Day 2

8:30 a.m.	The ONWI Presentation	
10:15	Break	
10:30	The NNWSI Presentation	
12:15 p.m.	Lunch	
2:30	The BWIP Presentation	
4:30	Executive Session	PANRG

Day 3

9:00 a.m.	Executive Session	PANRG
12:00 p.m.	Adjourn	

AGENDA

Performance Assessment National Review Group
Second Meeting: Flow and Transport Modeling
May 8-10, 1984
Rockville, Maryland

Day 1

9:00 a.m.	Greetings and Introductions	Lee
9:15	The BWIP Presentation	BWIPO/Rockwell
12:30 p.m.	Lunch	
1:30	The ONWI Presentation	SRPO/Battelle
4:30	Executive Session	PANRG

Day 2

8:30 a.m.	The NNWSI Presentation	NV/SNL/PNL
12:00 p.m.	Lunch	
1:30	Executive Session	PANRG

Day 3

8:30 a.m.	Executive Session	PANRG
12:00	Adjourn	

SUGGESTED OUTLINE OF PROJECT PRESENTATION TO PANRG
April 18-20, 1984

- Overall Plans to Demonstrate Compliance with 40 CFR 191 and 10 CFR 60

1. Overview of Project's Performance Assessment Program

2. Project's Interpretation of Compliance with 40 CFR 191.

3. Project's Interpretation of "Reasonable Assurance."

4. Which Scenarios Will Be Analyzed?

   How are they chosen?
   How will they be analyzed? [System Model]
   How will consequences be presented?
   How is uncertainty in these consequences treated?

5. How Will Probabilities be Associated with Scenarios?

6. How Will the Individual Probabilities and Consequences be Combined to Demonstrate Compliance? How Will the Results be Presented?

AGENDA

Performance Assessment National Review Group
Second Meeting
Gaithersburg, MD

Monday, July 9, 1984

8:00 a.m.	Greetings, Introductions and Ground Rules	Lee
8:15 a.m.	Tuff Source Term Presentation	NNWSI
9:15 a.m.	Questions and Discussion of Tuff Source Term Approach	PANRG
11:15 a.m.	Salt Source Term Presentation	ONWI
12:15 p.m.	Lunch	
1:00 p.m.	Questions and Discussion of Salt Source Term Approach	PANRG
3:00 p.m.	Basalt Source Term Presentation	BWIP
4:00 p.m.	Questions and Discussion of Basalt Source Term Approach	PANRG
8:00 p.m.	Executive Session	PANRG

Tuesday, July 10, 1984

8:00 a.m.	Defense High Level Waste Form Performance Assessment	SRL
8:30 a.m.	NRC Waste Package/Source Term Overview	NRC
9:00 a.m.	Discussion of General Approach to Source Terms	PANRG
12:00 p.m.	Lunch	
1:00 p.m.	Canadian Performance Assessment Overview	Lyon
1:30 p.m.	Tuff Radionuclide Transport Presentation	NNWSI
2:30 p.m.	Discussion of Tuff Transport Approach	PANRG
3:30 p.m.	Salt Radionuclide Transport Presentation	ONWI
4:30 p.m.	Discussion of Salt Transport Approach	PANRG
8:00 p.m.	Executive Session	PANRG

Wednesday, July 11, 1984

8:00 a.m.	Basalt Radionuclide Transport Presentation	BWIP
9:00 a.m.	Discussion of Basalt Transport Approach	PANRG
10:00 a.m.	Discussion of General Approach to Radionuclide Transport	PANRG
12:00 p.m.	Lunch	
1:00 p.m.	Tuff Geohydrologic Flow Presentation	NNWSI
2:30 p.m.	Discussion of Tuff Geohydrologic Flow Approach	PANRG
3:00 p.m.	Salt Geohydrologic Flow Presentation	ONWI
4:30 p.m.	Discussion of Salt Geohydrologic Flow Approach	PANRG
8:00 p.m.	Executive Session	PANRG

Thursday, July 12, 1984

8:00 a.m.	Basalt Geohydrologic Flow Presentation	BWIP
9:30 a.m.	Discussion of Basalt Geohydrologic Flow Approach	PANRG
10:00 a.m.	Discussion of General Approach to Evaluation of Flow	PANRG
11:00 a.m.	Discussion of Stochastic Hydrology	PANRG
12:00 p.m.	Lunch	
1:00 p.m.	Basalt Sensitivity and Uncertainty Analysis Presentation	BWIP
2:00 p.m.	Salt Sensitivity and Uncertainty Analysis Presentation	ONWI
3:00 p.m.	Tuff Sensitivity and Uncertainty Analysis Presentation	NNWSI
4:00 p.m.	Discussion on Sensitivity and Uncertainty Analyses Approaches	PANRG
8:00 p.m.	Executive Session	PANRG

Friday, July 13, 1984

8:00 a.m.	Executive Session
12:00 p.m.	Adjourn

Performance Assessment National Review Group
Request for Briefing

The Performance Assessment National Review Group (PANRG) is formed to review the development, documentation, verification, validation and application of mathematical models to predict the transport of radionuclides from the waste package, through engineered and geologic barriers, into the environment. The Projects are requested to provide PANRG specific information as outlined. To the extent possible, please summarize specifics and results, and provide information on the basis of these results sufficient for a technical person to follow up in more detail. This may include excerpts from reports and draft reports, references to specific parts of reports and publications, etc.

To the extent possible, please follow this general outline for the presentations to PANRG:

a. Present predictive techniques, including calculational methods:
   Identify computer codes or analytical approaches;
   Give mathematical formulations and key assumptions;
   Identify documentation, verification, benchmarking and validation plans and results; and
   Give input data, data sources and discussion of data validity.

b. Present currently available results and conclusions.

c. Discuss uncertainties in currently available results, analysis of such uncertainty, and plans for reducing such uncertainty.

d. Give plans for improvements in predictive techniques and codes and identification of data needs, data collection plans and prospective use of such data.

I. SOURCE TERM

PANRG plans to review the approaches and results for:

- determining waste package lifetime;
- compliance with the release rate criterion for the engineered barrier systems; and
- formulation of the source term for site subsystem analysis.

This review will consider the present state of knowledge on source terms and the way in which such knowledge is being used in connection with other related project work (e.g., contaminant analysis) for the various repository projects. It will also consider plans for developing source terms which will be sufficient for DOE decisions on repository plans and for NRC licensing.

"Source term" refers to the time-dependent rate of release of radionuclide species from the engineered barrier system. If any other definition or interpretation is used, please explain.

Topics for Presentations

1. Radionuclide Inventory

Give assumptions in terms of original fuel (MTHM) charged to the reactor regarding: waste mix and quantities, reactor burnup, time since discharge from the reactor, reprocessing, etc. Please provide assumed inventories of specific radionuclides at time of emplacement and at 10, 100, 1000, 10,000, and 100,000 years after emplacement.

2. Assumed or Reference Engineered Barrier System

- Loading per package (in terms of MTHM originally charged to the reactor)
- Waste forms (material, composition, and detailed description)
- Container/overpacks (materials, thicknesses, other details)
- Backfill or buffer materials (materials, dimensions, other details)
- Other relevant engineered components (detailed description of backfill, seals, and other components included in your definition of the engineered barrier system).

3. Waste-Package-Scale Environments

- Expected thermal environments (temperatures in waste form, in waste package components, and in very-near-field rock at time of maximum, at emplacement, and at 10, 100, 1000, 10,000 and 100,000 years after emplacement)
- Nuclear radiation environments that could affect performance
- Stress environments that could affect performance
- Fluid conditions assumed (water volume, replacement rate)

4. Waste Package Failure

- Failure modes considered for Waste Package and Engineered Barrier System.
- Corrosion Process (uniform, pitting, vapor, crevice, stress, grain boundary)
- Effect of Temperature
- Hydrogen Embrittlement
- Radiolysis
- Effect of Corrosion Products

5. Leaching

- Solubility
- Waste Form Dissolution
- Other Processes Affecting Leach Rates
- Leaching Products
- Extrapolation of Laboratory Data to Repository Conditions and Time Scales

6. <u>Radionuclide Transport</u>

Please discuss approach for predicting the species of radionuclides and other major chemical components (e.g., iron species) and their concentrations that might leave the waste form (container/overpack) and move into the backfill material. Discuss retardation effects, retardation data for key radionuclides, and the approach to prediction of radionuclide migration through the engineered barrier system. Discuss diffusion coefficients. Discuss effect of colloids and coordination complexes on transport. Discuss treatment of radioactive decay during transport.

7. <u>Chemical Processes</u>

Discuss techniques for predicting the chemistry of any water that might contact the container/overpack in the post-closure phase, and the groundwater chemistry evolution adjacent to the package as a function of time. Discuss prediction of the chemical form of the radionuclides and other chemicals. Discuss solubility data for key radionuclides. Discuss impacts of diffusion of oxidants, radiolysis products.

8. <u>Evaluation of Source Term for Site-Scale Transport Analyses</u>

Discuss how the spatial distribution of canisters within a repository, that may extend for kilometers, influences the formulation of the source term for the site subsystem analysis.

II. GROUND-WATER FLOW

PANRG will review the approaches to modeling flow on the regional and local scale which are used to evaluate:

- Fastest path and travel time to the accessible environment and

- Input information for the evaluation of radionuclide tranport.

The presentations should include details regarding the codes that will be used (viz., MAGNUM, PORFLO, SWENT or others) and the conceptual models to be used. The presentations should emphasize input data, results obtained, and validation.

On a regional scale, the presentations should discuss the conceptual models for the major sources of ground water and the information used to define the boundary conditions for the local-scale modeling. The local-scale modeling describes the flow in the vicinity of the repository including the effects of heat, partially-saturated flow, and interbed flow. The treatment of other sources of water at the sites (e.g., mineral dehydration) should also be discussed.

PANRG will also review the status of stochastic modeling of the hydrology. The presentations should discuss the extent to which these methods are being considered in the program and specific analyses that have been conducted or are contemplated.

III. RADIONUCLIDE TRANSPORT

PANRG is interested in the approaches and available results for the prediction of hydrogeologic transport of radionuclides, including:

- The cumulative releases of radionuclides to the accessible environment during the first 10,000 years after closure;
- Releases during the first 100,000 years;
- Time-dependent radionuclide concentration in major sources of ground water.

The following topics should be treated if they are relevant to a specific site.

- Evaluation of diffusion transport of radionuclides
- Formulation of dispersive transport in the transport equations, validity, dispersion coefficients, bases for dispersion coefficients, importance of dispersion in predicted results
- Data on chemical speciation, solubility, adsorption processes, effect of colloidal transport, ion exchange, isotopic exchange, uncertainties in such data and their integration into transport calculations
- Radionuclide diffusion into and out of dead-end pores
- Transport through and around repository seals and plugs

IV. UNCERTAINTY AND SENSITIVITY ANALYSIS

PANRG will review methods which are proposed for analyzing uncertainty and carrying out necessary sensitivity analyses for project guidance purposes and licensing. Presentations should include:

- Discussion of treatment of stochastic geohydrology;
- The approach and rationale for selecting the approach to other sensitivity and uncertainty analysis:
    - Monte Carlo
    - Latin Hypercube
    - Adjoint Method
    - Second-order Methods
    - Others

- Assumptions, details, and limitations in these approaches;
- Specific areas in which uncertainty and sensitivity analyses are contemplated;
- Whether different approaches are being considered for different specific areas;
- The extent to which calculations or analyses using bounding values may be appropriate in lieu of uncertainty analyses;
- Specific examples.

Appendix D

SIGN-IN SHEET

Wednesday, April 18, 1984

Name	Organization	Telephone Number
Ralph L. Keeney	Systems Science Department, University of Southern Cal.	415-391-4892
Bob Lyon	Atomic Energy of Canada Ltd.	204-753-2311
Stanley N. Davis	Dept. Hydrology & Water Res., University of Arizona	602-621-3131
David C. Kocher	Oak Ridge National Laboratory	615-576-2134
Philip E. LaMont	DOE-RL/BWIPO	509-376-6117
David H. Dahlem	DOE-RL/BWIPO	509-376-3022
Marc Wood	Basalt Waste Isolation Project, Rockwell	509-373-4013
Billy M. Cole	PNL-Washington, DC	202-785-6400
Leslie A. Casey	DOE/SRPO-Columbus, OH	614-424-5916
Carl Newton	DOE/HQ	301-353-4851
Carl Cooley	DOE/HQ	301-353-3014
Tom Pigford	University of California	415-642-6469
Bob Stern	DOE/HQ	202-252-4600
Larry Rickertsen	WESTON	301-963-6828
Abe Van Luik	WESTON	301-963-6842
Jack Ditmars	Argonne National Lab	312-972-3784
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Jack Parry	Battelle-ONWI	614-424-5090
Peter L. Hofmann	Battelle-ONWI	614-424-5683
David Dawson	Battelle-ONWI	614-424-9803

SIGN-IN SHEET (Continued)

Wednesday, April 18, 1984

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Jim Rollo	USGS-Director's Office	703-860-6082
M. D. Voegele	SAI/LV-NNWSI	702-295-1460
Felton W. Bingham	Sandia National Labs (NNWSI)	505-844-8816
George A. Dinwiddie	U.S. Gelogical Survey	703-860-6976
Donald Alexander	DOE/HQ	301-353-2431
David Michlewicz	EBASCO/ONWI	212-839-3225
Bill Owens	Consultant	918-494-3006
Marty Bensky	BWIP	509-376-7005 FTS 444
Donald Langmuir	Colorado School of Mines	303-273-3631
Bill Lee	WESTON	301-963-6812
David Siefken	WESTON	301-963-6817
Carol Hanlon	DOE/HQ	301-963-5200
Paul Gnirk	RE/SPEC	

ATTENDEES AT THE SECOND
PERFORMANCE ASSESSMENT NATIONAL REVIEW GROUP MEETING
GAITHERSBURG, MD
JULY 9-12, 1984

Name	Affiliation	Telephone
Tom Pigford	University of California	415-642-6469
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Name	Affiliation	Telephone
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John Randall	NRC/RES	301-427-4633 FTS 427-4633
Lyn Ballou	LLNL	FTS 532-4911

Name	Affiliation	Telephone
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Cyrus Klingsberg	DOE/HQ	FTS 233-353-3227
Tim Johnson	NRC/WM	301-427-4088
George Jansen	BMI/ONWI/PAD	FTS 976-7317
G. E. Raines	BMI/ONWI	FTS 976-7832
Lake Barrett	NRC	FTS 427-4119
John Greeves	NRC	FTS 427-4612

UNITED STATES
NUCLEAR REGULATORY COMMISSION
WASHINGTON, D.C. 20555

SEP 10 1984

Mr. William Bennett
Acting Associate Director
Office of Geologic Repository Deployment
Office of Civilian Radioactive
  Waste Management
Department of Energy
Washington, DC 20554

Dear Mr. Bennett:

At the Performance Assessment National Review Group (PANRG) meeting held in Gaithersburg on July 9 to July 12, 1984, it came to our attention that there was confusion over the requirements for release of radionuclides from the engineered barrier system. At the meeting we indicated we would clarify our position.

The rule, 10 CFR Part 60, states:

(§60.113(a)(1)(ii)(B))

> The release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years following permanent closure, or such other fraction of the inventory as may be approved or specified by the Commission; provided, that this requirement does not apply to any radionuclide which is released at a rate less than 0.1% of the calculated total release rate limit. The calculated total release rate limit shall be taken to be one part in 100,000 per year of the inventory of radioactive waste, originally emplaced in the underground facility, that remains after 1,000 years of radioactive decay.

The confusion at the PANRG meeting related to the method of computing the 0.1 percent of the total release rate for the exempted radionuclides. We have attached an example calculation which clarifies our intent.

If you have any questions, please contact Mr. Lake H. Barrett, at (FTS) 427-4173 or myself at (FTS) 427-4069.

Sincerely,

Robert E. Browning, Director
Division of Waste Management

Enclosure

SEP 10 1984

CALCULATION OF I-129 RELEASE RATE

PURPOSE

The purpose of this calculation is to determine the required I-129 release in accordance with the 10 CFR Part 60 engineered barrier system requirements for the Nevada Nuclear Waste Storage Investigations (NNWSI).

REFERENCES

1. 10 CFR Part 60, "Disposal of High-Level Radioactive Wastes in Geologic Repositories."

CALCULATION

The rule, 10 CFR Part 60 (Ref. 1), states release rate requirements for the engineered barrier system for a high-level waste repository. These release rate requirements are given below (§ 60.113(a)(1)(ii)(B)).

> The release rate of any radionuclide from the engineered barrier system following the containment period should not exceed one part in 100,000 per year of the inventory of that radionuclide calculated to be present at 1000 years following permanent closure, or such other fraction of the inventory as may be approved or specified by the Commission; provided, that this requirement does not apply to any radionuclide which is released at a rate less than 0.1% of the calculated total release rate limit. The calculated total release rate limit shall be taken to be one part in 100,000 per year of the inventory of radioactive waste, originally emplaced in the underground facility, that remains after 1000 years of radioactive decay.

This requirement allows radionuclides which have very low inventories to be exempt from the 1 part in 100,000 annual release rates.

I-129 is a nuclide which will have a low curie inventory at 1000 years relative to the total inventory in the repository. This calculation will determine if the I-129 inventory in spent fuel will allow it to be exempted from the 10 CFR Part 60 individual radionuclide release rate requirement of 1 part in 100,000.

Table 1 provides a nuclide inventory for spent fuel for the NNWSI repository project. The total inventory at 1000 years is computed from the data in Table 1 and is 17.6×10^5 uCi/kg U. This value is based on a 33 MWd/kg U burnup. The I-129 inventory at 1000 years is given as 32 uCi/kg U.

In order for I-129 to be exempted it must be released at a rate less than 0.1 percent of the total release rate. The total release rate will be:

$$17.6 \times 10^5 \text{ uCi/kg U/yr } \left(\frac{1}{10^5}\right) = 17.6 \text{ uCi/kg U/yr.}$$

In order for I-129 to be exempted from the 1 part in 100,000 annual release rate criteria, it must have a release rate of less than $(17.6 \text{ uCi/kg U/yr})(10^{-3}) = 0.0176$ uCi I-129/kg U/yr.

If it is assumed that all the I-129 is released in one year, it will be released at a rate of:

32 uCi/kg U/yr.

Therefore, the I-129 cannot be summarily dismissed because this maximum annual rate of release exceeds 0.0176 uCi/kg U/yr. If, however, release rate information for I-129 can be obtained which shows that the maximum annual release rate will not exceed 0.0176 uCi/kg U/yr, I-129 could be dismissed from further consideration. For this second option to occur, a release rate fraction of less than:

$$\frac{0.0176 \text{ uCi/kg U}}{32 \text{ uCi/kg U}} = 5.5 \times 10^{-4}.$$

would have to be demonstrated. This value, however, would be less restrictive than the 1 in 100,000 release value which would otherwise be required.

Calculated By [signature] 9-6-84
Checked By John M. Greeves 9-6-84
Approved By [signature] 9/6/84

SPENT FUEL RADIONUCLIDE CONTENT* IN ORDER OF DECREASING ACTIVITY AT 1000 YEARS (33 MWd/kg U PWR Fuel)

Radionuclide	μCi/kg U at Years from Discharge[10] 10 yr	1000 yr	10,000 yr	Half-Life[11] (years)
^{241}Am	1.7×10^6	9.3×10^5	10.6	458
^{240}Pu	5.3×10^5	4.8×10^5	1.9×10^5	6580
^{239}Pu	3.2×10^5	3.1×10^5	2.4×10^5	24,400
^{243}Am**	1.7×10^4	1.6×10^4	7.0×10^3	7370
^{99}Tc	1.4×10^4	1.4×10^4	1.3×10^4	2.1×10^5
^{93}Zr	3.0×10^3	3.0×10^3	3.0×10^3	1.5×10^6
^{234}U	1.2×10^3	2.0×10^3	2.0×10^3	2.5×10^5
^{242}Pu	1.9×10^3	1.9×10^3	1.8×10^3	3.8×10^5
^{14}C***	1.5×10^3	1.4×10^3	4.6×10^2	5730
^{238}Pu	2.2×10^6	1.0×10^3	--	86
^{237}Np	3.3×10^2	1.0×10^3	1.2×10^3	2.1×10^6
^{126}Sn	8.0×10^2	8.0×10^2	7.5×10^2	$\sim 10^5$
^{79}Se	4.2×10^2	4.2×10^2	3.8×10^2	6.5×10^4
^{135}Cs	3.8×10^2	3.8×10^2	3.8×10^2	3.0×10^6
^{151}Sm	3.6×10^5	2.3×10^2	--	93
^{107}Pd	1.2×10^2	1.2×10^2	1.2×10^2	7.0×10^6
^{129}I	32	32	32	1.7×10^7
^{241}Pu	8.0×10^7	21	10	13
^{230}Th	0.1	16	164	8.0×10^4
^{226}Ra****	3.3×10^{-4}	3	128	1600
^{210}Pb	4.0×10^{-5}	3	128	--

*Includes radionuclides with half-lives greater than 1 year and with activities greater than 10^{-8} of total 1000-year activity.

**^{243}Am decay followed by 2-day half-life ^{239}Np daughter product decay.

***^{14}C activity will vary depending on initial fuel nitrogen content.

****Relatively rapid (~22 year) eight-step decay chain from ^{226}Ra to stable ^{206}Pb, only ^{210}Pb in this chain has a half-life greater than 1 year.