NUCLEAR WASTE CONSULTANTS INC.
8341 So. Sangre de Cristo Rd., Suite 6
Littleton, Colorado 80127
(303) 973-7495

February 15, 1986 '86 MAR -3 P4:42

009/5/Meetings.001
RS-NMS-85-009
Communication No. 26

U.S. Nuclear Regulatory Commission
Division of Waste Management
Geotechnical Branch
MS 623-SS
Washington, DC 20555

Att: **Mr. J. Pohle, Project Officer**
Technical Assistance in Hydrogeology - Project B (RS-NMS-85-009)

Re: **Trip Report:**
Attendance at Workshop on "Validation of Mathematical Models for Waste Repository Performance Assessment - Confidence Building Through Synthesis of Experiments and Calculations"
January 27-29, 1986

Dear Mr. Pohle:

Please find attached Nuclear Waste Consultants, Inc.'s trip report for Adrian Brown's attendance at the workshop on "Validation of Mathematical Models for Waste Repository Performance Assessment - Confidence Building Through Synthesis of Experiments and Calculations", held in Bethesda, Maryland on January 26 through January 29, 1986.

The conclusions of this trip report are that there appears to be a general lack of direction in the research program as described in this workshop, which has resulted in much of the research that is currently underway being directed at areas that are not apparently of critical importance to the program, while other critical areas are currently left unresolved and unresearched. This difficulty would have to be resolved before it would be possible to reach any useful consensus on the need for validation of models, which was the stated purpose of the workshop.

If you have any questions about this report, please do not hesitate to contact the undersigned or Mark Logsdon.

Respectfully submitted,
NUCLEAR WASTE CONSULTANTS, INC.

Adrian Brown

Adrian Brown, Project Director

Att: Trip Report

cc: US NRC - Director, NMSS (Attention: PSB)
DWM (Attention: Division Director)
Barry Bromberg, Contracting Officer
WMGT (Attention: Branch Chief)

2890

TRIP REPORT

WORKSHOP ON VALIDATION OF MATHEMATICAL MODELS - JANUARY 27-29, 1986

1.0 INTRODUCTION

At the request of the Project Officer for Project RS-NMS-85-009, Adrian Brown attended a workshop entitled "Validation of Mathematical Models for Waste Repository Performance Assessment - Confidence Building Through Synthesis of Experiments and Calculations" which was held in Bethesda, Maryland, on January 27 to January 29, 1986. The workshop was sponsored by the U.S. Nuclear Regulatory Commission's Office of Nuclear Regulatory Research, and was organized by Sandia National Laboratories. The workshop is one of a series that are planned to address issues in the validation of modeling used for prediction of the performance of high-level waste repositories.

The agenda and the background material for the meeting are attached to this report as Appendix A.

2.0 OBJECTIVE OF THE WORKSHOP

The overall objective of the workshop series is stated as "... to build confidence in mathematical models used to describe coupled and uncoupled processes over the several length and time scales important to repository operations." (Supporting document, page 3).

It was stated on page 7 of the supporting document that (presumably as a result of these workshops) "..NRC hopes to achieve a basis for decisions in the following areas:

- o Design of field tests appropriate for model validation and development.
- o Determination of the kinds of laboratory experiments to be conducted.
- o Identification of mathematical models in need of validation.
- o Identification of problems that need to be solved.
- o Identification of the kinds of natural analogue systems that can be used to validate mathematical models."

These objectives seem to be entirely reasonable, and have the potential to form the basis for a most worthwhile workshop.

The objective of this first workshop appeared to be to develop an understanding of "... the confidence that can be placed in results obtained from mathematical models used in performance assessment methodologies." (Supporting document, page 6). There appeared to be some lack of clarity as to this objective, as a later attempt at a firmer definition of the purpose for the participants attending the workshop was attempted in these terms:

> "For each spatial scale, the task for workshop participants is to determine time scales of importance to repository performance." (Supporting document, page 8).

3.0 PROGRAM

The program was as described on the agenda, which is attached as part of Appendix A. The first day was given over to an evaluation of validation of models of the performance of the thermally undisturbed zone, the second day evaluated validation of models of the thermally disturbed zone, and the last day (which was not attended by Mr. Brown) was reserved for a discussion of validation of modeling of the performance of the waste package.

Each day involved a series of presentations by persons considered by the organizers to be leaders in the appropriate fields, with essentially no comment time available during the presentations. At the end of these presentations, a half hour discussion period was allowed before lunch. After lunch, two hours were allowed for panel "discussions", which were in fact additional presentations by the panel members, generally pre-prepared and usually unrelated to the presentations of the morning. A limited amount of time was available for floor involvement in these discussions and presentations. Finally, each day's session ended with an attempt to "build consensus" about needed experiments for the validation of the models that were discussed during the day.

3.1 NATURAL BARRIERS - THERMALLY UNDISTURBED ZONE

The presentations made during this part of the program were:

1. Hydrocoin Program - Paul Davis, Sandia. Paul presented the present status of the Hydrocoin program, which appears to be an international effort to provide calibration and/or validation opportunities for models being used by the international waste disposal community.

2. Transport Phenomena - Lynn Gelhar, MIT. Dr. Gelhar gave a talk on the current state of the art with respect to dispersion. He evaluated dispersion using "equations we all believe in", and apparently reached the conclusion that there are only a few field experiments that have ever been conducted to evaluate dispersion that meet his standards of academic rigor. Accordingly, he essentially discounts all studies of dispersion at scales greater than as few tens of meters. Little of Dr. Gelhar's discussion related to validation or models.

3. Hydrology - Shlomo Neuman, Arizona. Shlomo gave a well presented description of validation exercises. His main example was of the modeling of piezometric response in sediments adjacent to a river to flooding of the river. The response to an initial flood was used to determine values for the hydraulic parameters of the materials, based on a reasonable fit between observed and predicted responses. The model was then used to predict the response to a second flood, which it did admirably. However, as Dr. Neuman pointed out, this exercise was hardly "validation" in its strictest sense, as the parameters arrived at for the various layers in the system might not constitute a unique system.

4. Geochemistry - Malcolm Siegel, Sandia. Malcolm began his presentation by giving the Ziegler (1976) description of validation, based on replicative, predictive, and structural validation, which appears to be a useful approach. He then went on to describe a list of validation exercises that were, in his opinion, needed to allow geochemical modeling (in general) to advance to the point where it would be of utility in the high level program.

The panel discussion in the afternoon, seemed to mainly provide an opportunity for participants to present some further ideas, often not obviously linked to the subject of the workshop, followed by a response by the moderator. Jaak

Daemen and Doug Vogt gave some direction to the workshop by asking how much of what we heard during the morning related to an ongoing program for validation.

Following the panel discussion, there was a presentation on the Intraval program, which was described as an extension of the international effort to arrive at validation of models including the interaction between heat, chemistry, and hydraulics. It is in its formative stages at this time.

Finally, the participants were asked to review the questions that had been circulated previously (Appendix A, page 10 and 11). As no connected statement had previously been presented of the status of the research program being funded by the NRC, it proved impossible for the participants to seriously address such questions as "What are the important transport processes in this spatial domain?" and "What are the major sources of uncertainty in understanding and modeling radionuclide transport?" and "How can the validity of the above assumptions be tested?"

3.2 NATURAL BARRIERS - THERMALLY DISTURBED ZONE

The second day's activities focussed on the area closer to the repository. The talks presented were as follows:

1. Hydrology (saturated media) - Paul Davis, Sandia. Paul presented several validation efforts that have been performed in order to increase assurance that coupled heat/flow/stress/transport codes effectively model the relevant coupled phenomena. The conclusion of his presentation is that these validation efforts are in their infancy, and that there has to date been no published validation at a

field scale of coupled modeling of heat, flow, and transport, nor of stress, flow, and transport.

2. Hydrology (unsaturated media) - Kirsten Preuss, Lawrence Berkley Laboratories. Dr. Preuss presented a paper on the flow behavior in and immediately adjacent to a single fracture in partially saturated tuff, under thermal conditions similar to those expected near a cannister. The conclusion of the paper appeared to be that the fluid transport mechanism involved evaporation, vapor transport, cooling, condensation, and unsaturated groundwater flow. The extent to which this mechanism has the potential to transport radionuclides, or the extent to which this mechanism might be of significance to the performance of a repository in unsaturated tuff has apparently not yet been addressed. However Dr. Preuss indicated that the processes that he was examining were "extremely sensitive to molecular levels of water on fracture walls."

3. Geochemistry - Don Langmuir, Colorado School of Mines. Dr. Langmuir presented a discussion of his view of the state of the art with respect to the transport of radionuclides in geologic media. He stated that the thermodynamics of the transport of uranium, radium, and thorium are relatively well known, while the behavior of most of the remainder of the artificial radionuclides was relatively inexactly known. He questioned the use of Kd as a tool in the program, mainly on the grounds that validation of transport problems using solely Kd approaches was likely to be unsuccessful. He presented a graph showing all the results for the Kd of Neptunium V which showed enormous scatter (more than 6 orders of magnitude), as an example of the uncertainties remaining in the program.

4. Geomechanics - Tsang Chin Fu, Lawrence Berkley Laboratories. Dr. Tsang (standing in for Dr. Noorishad) provided an update on the state of coupled geomechanical/thermal/hydrological/geochemical modeling, and of the validation of such modeling. It was his conclusion that the present codes are in a "primitive" state of development, and that a vast amount of code development would be required before useable codes were developed for the high level program. He also concluded that meaningful validation for such models was extremely difficult.

5. Geomechanics - Charles Fairhurst, University of Minnesota. Dr. Fairhurst presented the results of two actual validations of codes that are proposed for use in the high level program. The main example he used was the validation of the discrete element code UDEC using the results of the BWIP block test in the NSTF. This was a "pure" validation, in that the results of constitutive relationships developed from small sample tests of the materials and the joints were used in the modeling activity, the loads applied, and the

deflections predicted. These predictions were found to be in good agreement with the observations.

The discussion following in the afternoon concentrated heavily on the Kd issue, with considerable interplay between those who saw the issue as one of the use of an approach to contaminant transport that ignored the fundamental physics of the situation, and was thus unlikely to be capable of validation, versus those who saw the Kd approach as providing a useful shorthand way of lumping a wide range of complex processes into one empirical relationship.

As on the previous day, the participants were asked to provide guidance on the needed research in the area of model verification for support of HLW performance assessment. Again, this was found to be a difficult undertaking in the absence of an evaluation of the needs of the program by license time, a review of the present status of the research program, and some attempt by any of the speakers to define the most pressing needs in their topic areas.

4.0 EVALUATION OF THE WORKSHOP

In the opinion of this participant, this workshop was both timely and necessary, and had the potential to make a significant contribution to the NRC's research program, for the following reasons:

1. There will always be a need for communication between the people planning and performing research and the people using the results of that research.

2. In the HLW program, the NRC still has a wide range of critical research needs, in order to be positioned by license time to respond to a license application in order to fulfil its mandate. Specifically, with respect to research into matters of far and near field hydrology, the NRC certainly needs to have access to the results of research into fluid flow and radionuclide transport, and the way in which these transport mechanisms are influenced by stress and temperature. The question is, how much research, directed into which particular area of these extremely broad categories, and conducted in which way?

3. Time for the research is short, and the budget for such research is far from infinite, so that the NRC is faced with a resource allocation problem. Who better to seek advice from than a mixture of the people that will ultimately perform the research, and the people that will ultimately sink or swim using the results.

Unfortunately, in the opinion of this participant, the workshop fundamentally failed in its aims. The following paragraphs indicate the areas in which the workshop appeared to be a problem:

1. Lack of agreement on basic analytical needs. In order to decide the needs for validation of computer codes, it is first necessary to decide on which computer analyses are needed. This participant considers that many of the analytical tools that are under development today are unnecessary in the context of the HLW program, as the data needed to drive them and the validation needed to allow their use in the program are essentially unobtainable within the time and access constraints that operate in the program. Until some

evaluation is made of the analyses that actually must be made by or for the NRC for it to do its job, then discussions such as took place in Bethesda will be essentially futile.

2. Tendency to code development rather than problem solution. There are a wide range of codes available today for the analyses that probably need to be performed for the reasonable evaluation of the impact of a HLW repository on human health and safety. However it is in general easier for a research organization to develop new and more complex codes than it is to grapple the problem of what, as a minimum, is needed for HLW license decision making.

3. Tendency to focus on the interesting technical problems, rather than the critical technical problems. This participant to the workshop considers that the primary licensing decisions that must be made by the NRC will be made based on relatively simple, uncoupled evaluations of the far field barrier, together with relatively complex, intensive evaluations of the performance of engineered barriers within the repository. It does not seem likely, given the time or funds available, that the NRC or the DOE will disentangle the behavior of the near field rock (the thermally disturbed zone) sufficiently to allow much credit to be taken for it in either transit time or radionuclide flux computations. Despite this, a very considerable amount of research effort appears to be being devoted to developing and validating codes that attempt to couple the complex and poorly understood relationships between stress, flow, and heat. This effort appears to this participant as fascinating, but unnecessary and probably unusable in a licensing context.

4. Microscopic concentration of researchers. In much of the program that was presented in the workshop, there was a microscopic rather than a macroscopic focus. There are two philosophical ways to discover how a system works, and hence to be in a position to predict its future behavior.

   a. The "take it apart and test the components" approach. In this approach, the investigator pulls the system to pieces, evaluates the behavior of each piece in as much detail as possible, re-assembles the pieces in some kind of analog, applies the same stimuli to the analog as are expected in the real situation, and observes the results. In order for this process to allow much confidence in the results of the prediction, there is a need for validation of the end result by comparing the results of the evaluations with some known situation. This is the approach that is almost universally being adopted by the HLW program, which explains the great need for validation.

b. The "direct system evaluation" approach. In this approach, a model of the system is developed as rationally as possible, but it is considered to be a "black box". Testing of the system is performed by applying stimuli to the real system at as close to full scale and as close to a direct analog of the real repository system as possible. The model of the system is then calibrated using the prototype results as a guide. In general this process provides a set of parameters for the components of the model, some of which can be directly measured to provide a measure of validation of the model. The predictive process becomes an extrapolation of the prototype test(s), more than an open traverse into the future.

Ideally, a practical HLW repository performance evaluation would be a combination of both these approaches, with the resulting confidence created by a calibrated, verified model. Practically, in some of the sites there is no opportunity to stress the system at the scale needed for the system approach, and in others there is no ability to test the components sufficiently to define them. Thus the approach that is needed is site and material specific. Because of this, the current research program approach (the "take apart and test the components" approach) is not likely to be effective on at least some of the sites under consideration.

5. Lack of agreement as to what constitutes validation. Before a discussion of validation of models could be reasonably attempted, it would be necessary to define the term. There seemed to be a considerable divergence of opinion at the workshop as to the meaning of many of the terms used in the evaluation of the utility of a computer or analytical tool. Terms that would appear to require sorting out include verification, validation, and calibration. For the record, this participant considers that the following concepts are a reasonable starting place for these definitions:

   a. Verification. Establishing that a computer or other process correctly performs the computations that the algorithm calls for.

   b. Calibration. Determining or refining the parameters that describe the behavior of the components of a system based on the match between the observed behavior of the real system and the behavior of the model under the same or similar stimuli.

   c. Validation. Demonstration of an independent match between the predicted responses to a set of stimuli developed by a modeling exercise, and the observed responses of a real system to the same stimuli.

It is the independence factor that sets calibration apart from validation.

In summary, there appeared to be a general lack of central direction in the research program as described in this workshop, which has resulted in much of the research that is currently underway being directed at areas that are not apparently of critical importance to the program, while other critical areas are currently left unresolved and unresearched. This difficulty would have to be resolved before it would be possible to reach any useful consensus on the need for validation of models.

5.0 SUGGESTIONS FOR DESIGN OF A RESEARCH NEEDS ASSESSMENT WORKSHOP

It is the observation of the participant that it is considerably easier to be critical of an activity than it is to be constructive. Accordingly, the notes below have attempted to set out the aims that would appear to be appropriate for a research program in support of the NRC's HLW program, and the outline of a research workshop that might have a reasonable prospect of evaluating the current movement towards satisfaction of those aims. The orientation of the approach is unashamedly that of a person or group charged with the responsibility of reviewing a license application.

5.1 AIMS OF A RESEARCH PROGRAM IN SUPPORT OF THE NRC'S HLW REPOSITORY PROGRAM

Research in support of the NRC's HLW program should presumably be directed at the needs of the program. This is distinct from "pure" research, the funding for which should come from sources that are empowered to advance the general state of knowledge, for example the National Science Foundation.

The research needs of the NRC's HLW program are to resolve those theoretical and practical questions that are presently unresolved and that require resolution prior to the evaluation of a HLW repository license. Accordingly, only those questions for which resolution is considered to be needed, which remain unresolved, and which appear to be adequately resolvable within the timeframe of the HLW program should receive funding.

5.2 AN APPROACH TO THE EVALUATION OF RESEARCH NEEDS

Using the above objective of research, research needs can be evaluated by a reasonable process:

1. An overview of the possible processes that might affect the performance of a HLW repository system would be prepared.

2. Simple bounding calculations would be prepared to identify the extent to which each process was likely to be important with respect to the performance of the repository (note that this would likely be a site specific evaluation, as important processes at one site might well be entirely different from those at another).

3. The impact of each process on the uncertainty in the overall performance evaluation of the repository would be evaluated, based on the current knowledge of the process and the parametric information available to drive the evaluation of that process.

4. The uncertainty associated with the process under consideration would be divided into theoretical uncertainty (that is uncertainty about the process itself) and parametric uncertainty (that is uncertainty in the parameters that are needed to evaluate the process). The former is largely a matter for research, the latter is largely a matter for investigation.

5. Research needs for the process under consideration would be evaluated, assuming that there were no competing needs to be considered.

6. The research needs for all the processes would be assembled, and ranked in order of the extent to which the resolution of these research needs would produce needed improvement in the ability to evaluate the performance of a repository.

7. The ranked list would be scanned to eliminate those items for which the needed resolution is deemed to be impossible within the time or fiscal constraints of the program.

8. The remaining list is the ordered list of research priorities.

5.3 TENTATIVE DESIGN OF A WORKSHOP FOR EVALUATION OF HLW RESEARCH NEEDS

A workshop could be profitably organized that would assist the NRC in identifying the remaining research needs, and to define worthwhile research projects to address those needs, as follows:

1. Commission a study or a series of studies (one at each contending site) to identify the research needs for each site on a discipline by discipline basis, using the approach outlined above.

2. Have the results of these research needs evaluations presented as the opening activity of a workshop, to which a wide range of representatives of eligible research organizations and other members of the technical community would be invited (if possible, circulate the results beforehand, so that the participants could be informed when they arrive).

3. Use the workshop as a forum to evaluate the reasonableness of the results of the studies presented, the perceived need for the identified research, and the chances of success of the identified research.

The outcome of the workshop could be the development of a consensus program for further critical research that the NRC should consider funding. Such a research needs evaluation could be drawn as widely or as narrowly as the NRC would wish.

APPENDIX A

WORKSHOP ON VALIDATION OF MATHEMATICAL MODELS FOR WASTE REPOSITORY PERFORMANCE ASSESSMENT - CONFIDENCE BUILDING THROUGH SYNTHESIS OF EXPERIMENTS AND CALCULATIONS

AB DOC 1 1/27/86

January 27 - 29, 1986 - Washington, D.C.

Sponsored by the

U.S. Nuclear Regulatory Commission

Office of Nuclear Regulatory Research

Organizers:

E. J. Bonano
Waste Management Systems
Division 6431
Sandia National Laboratories
Albuquerque, New Mexico 87185
Tel: 505-844-5303

F. A. Kulacki
College of Engineering
Colorado State University
Fort Collins, Colorado 80523
Tel: 303-491-6603

J. D. Randall
Waste Management Branch
Division of Radiation Programs
& Earth Sciences
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
Tel: 301-427-4633

WORKSHOP ON VALIDATION OF MATHEMATICAL MODELS FOR WASTE REPOSITORY PERFORMANCE ASSESSMENT - CONFIDENCE BUILDING THROUGH SYNTHESIS OF EXPERIMENTS AND CALCULATIONS

Proceedings:	All presentations and discussion sessions will be tape-recorded and transcribed. An edited version with illustrations and vu-graphs will be published in a NUREG-CR report to be issued by Sandia National Laboratories early in 1986. This report will serve as a starting point for a second workshop to be held in spring 1986.
Follow-Up Workshop:	Tentative Time - April 1986
Place:	Washington, D.C.
Goals:	Review of recommendations of the first workshop on future research needs for validation of mathematical models.

WORKSHOP ON VALIDATION OF MATHEMATICAL MODELS FOR WASTE REPOSITORY PERFORMANCE ASSESSMENT - CONFIDENCE BUILDING THROUGH SYNTHESIS OF EXPERIMENTS AND CALCULATIONS

OVERVIEW

The NRC has organized this series of workshops to address the validation of models and their assumptions for high-level (HLW) repository performance and assessment. The conceptual framework is the prediction of results from controlled laboratory experiments and/or well-documented field studies. Achieving validation is viewed as an iterative process through which existing models are used to identify and define necessary laboratory and field experiments which are then used to improve the models themselves.

The overall goal of these workshops is to build confidence in mathematical models used to describe coupled and uncoupled processes over the several length and time scales important to repository operations. Essentially, these workshops will provide NRC with a tentative future agenda for research. Additionally, workshops such as these are timely owing to the continuing need to integrate effectively NRC-sponsored research programs and to provide researchers developing mathematical models with realistic and attainable validation procedures.

Objectives of the workshops will proceed from problem definition to setting expectations and precision of predictive models. Sensitivity and system analyses will be major elements in model validation, as will quantification of experimental uncertainties in both laboratory and field work. Code validation activities resulting from recommendations made at these workshops should complement benchmarking calculations, such as done in the Hydrocoin program. The basis for recommendations for future experiments and model validation will be developed from position papers by experts in the scientific disciplines relevant to disposal of HLW, as well as condensed reports of recent and ongoing research.

RATIONALE

The NRC is currently conducting research related to assessing the performance of HLW repositories which will be built and operated by the U.S. Department of Energy (DOE). The waste form for initial repositories will be both spent fuel (SF) and HLW; candidate host rocks at this time are salt, tuff, basalt, and granite. Siting and licensing of a repository depends on a host of technical issues that generally are being researched by NRC, DOE, EPA, national laboratories, universities, and industry. These combined programs are building the technical basis for NRC's independent assessment of proposed repository designs and geologic locations.

A major part of current NRC research is the development of overall methodologies to assess repository performance and its impact on a future human population or individual. These methodologies consist of mathematical models which estimate the impact of the repository on the geologic environment and the effects of the environment on the integrity of the waste package. Several models, some embodied in computer codes, have been developed to describe the various interactions of a repository with the local and regional environments with varying degrees of complexity. Thus far, a comprehensive mathematical model has yet to be developed for predicting all of the thermal, hydrological, mechanical, and chemical interactions of the repository with its geologic environment. Predictions are typically made on a subset of interactions, i.e., those considered as either "strong" or of special interest for a given host rock, time scale, and spatial scale.

Key elements of NRC research are laboratory and field experiments to evaluate and characterize overpack, packing, and backfill materials; field tests at potential candidate repository sites and at natural analog sites; and controlled laboratory experiments for specific transport processes relevant to model development and validation. Each of these experimental programs brings with it a degree of imprecision in the results arising from normal experimental error, selection of field test sites, and the limitations of modelling in the laboratory all of the complex conditions that will exist in a repository site.

These unavoidable shortcomings in both modelling and experimentation ultimately lead to questions of the accuracy and precision needed in predictions from mathematical models used in performance assessment. The underlying assumptions of such models must also be brought under scrutiny. The NRC

believes that the time is right for bringing together experimentalists and mathematical modellers to build a basis and consensus for confidence in predictions, as well as to develop "design-base" experiments for model development and validation.

TECHNICAL BASIS

The issues to be addressed in this workshop relate to the confidence that can be placed in results obtained from mathematical models used in performance assessment methodologies. These are grouped into the following categories:

Site Characterization

- How does one characterize a proposed site for analysis?
- What assumptions and data are needed at a proposed site to provide input parameters to mathematical models?

Appropriate Complexity of Analysis

- What is the appropriate complexity or detail needed for a given site, e.g., integral scale versus finite-difference methods?
- At what point does one compromise between the precision needed in spatial scale, time scale of application of results, and inaccuracies of input data?
- What couplings should be considered between thermal, hydrological, mechanical, and chemical processes for a given site, spatial scale, and time scale?
- What role should approximate analysis play in providing "bounding" estimates of coupled effects in addition to full numerical treatment of the problems?

Definition and Use of Laboratory Experiments

- How does one define and design controlled laboratory experiments suited to model validation?
- How does one develop simulant materials and laboratory samples to replace typical repository environments in experimental work?
- How much information is required to assure that laboratory experiments are dynamically similar to a potential repository site?

- To what extent can laboratory studies with real or simulant materials be used to provide input data or rate relations for mathematical models?

Definition and Use of Field Tests

- What are the appropriate criteria to be applied in designing a field test program?
- What time and length scales are appropriate for a field test program?
- What inaccuracy can be tolerated in field test results and yet be acceptable for validation of mathematical models?
- What experimental procedures assure dynamic similarity of field tests with a repository?

Definition and Use of Natural Analogues

- What are appropriate criteria for identifying useful natural analogues?
- What spatial scales are appropriate for natural analogues relative to anticipated repository size?
- What uncertainty level is permissible in describing the history of a natural analogues?
- What information is required from field tests to assure that natural analogues are dynamically similar to a potential repository?

Out of the answers to these and related questions on repository licensing, NRC hopes to achieve a basis for decisions in the following areas:

- Design of field tests appropriate for model validation and development.
- Determination of the kinds of laboratory experiments to be conducted.
- Identification of mathematical models in need of validation.
- Identification of problems that need to be solved.
- Identification of the kinds of natural analogues systems that can be used to validate mathematical models.

Related technical and scientific questions must be viewed on the appropriate time and space domains. The physical state of the repository and its geologic environment can be viewed as being determined at discrete points in time. A sequence of such descriptions forms the performance history of the repository and its geologic impacts. Achieving such a description, however, requires that the spatial and temporal elements of the overall problem of containing ionizing radiation in accordance with federal regulations be discretized to obtain well posed, tractable problems for mathematical modelling and/or experimentation.

For temporal and spatial scales, the definitions shown in Tables 1 and 2 will be used to focus discussion on problems and the status of their solution in the several spatial sub-domains of the repository region.

For each spatial scale, the task for workshop participants is to determine time scales of importance to repository performance. To facilitate discussion, each spatial sub-domain will be defined, and several assumptions will be made on initial and/or boundary conditions for nuclide release and transport processes. A series of questions for discussion is then posed for speakers and panelists to give the workshop a framework for reaching a consensus.

Table 1

Approximate Time Scales for Various Periods of Repository Operation

Repository Period	Time (y)
Construction & Operation	0 - 50
Closure & Containment	
- Thermally Active	30 - 500
- Thermally Inactive	500 - 1000
Controlled Release & Transport	500 - 10,000
Very Large Time	> 10,000

Table 2

Spatial Domains Associated with a Repository

Barrier	Spatial Domain
Natural	Thermally Undisturbed Zone
Natural	Thermally Disturbed Zone
Engineered	Repository Facility
Engineered	Waste Package

NATURAL BARRIERS - THERMALLY UNDISTURBED ZONE

Definition

The thermally undisturbed zone is that geologic domain where thermomechanical and geochemical effects of the repository facility and waste are not significant. This zone extends to the boundary of the accessible environment as specified by the EPA Standard (40CFR191).

Assumptions

1. The initial state is the ambient geologic setting when containment has failed. — PESSIMISTIC
2. The time-dependent concentration flux at the inner boundary is given.
3. Radionuclide concentrations are sufficiently low so that water density is unaltered.
4. The use of Kd's is acceptable.
5. Adsorption is the only important radionuclide retardation mechanism.
6. Low-temperature (25°C) geochemical data are adequate for modelling.
7. Steady-state hydrology and geology exist.

Questions for Speakers and Panelists

1. What are the important transport processes in this spatial domain?
2. Are all important couplings among these processes being considered?
3. What criteria should be used to establish the relative importance of a transport process?
4. What are the major sources of uncertainty in geochemical, geomechanical, geothermal, and hydrologic data that will potentially affect radionuclide transport?
5. What are the major sources of uncertainty in understanding and modelling radionuclide transport?

6. How does one bound radionuclide transport at this spatial scale? What modelling and experimental techniques should be used?

7. How can the validity of the above assumptions be tested?

NATURAL BARRIERS - THERMALLY DISTURBED ZONE

Definition

The thermally disturbed zone is that region where thermomechanical, geochemical, and hydrological effects of the repository are significant.

Assumptions

1. The initial state of the geologic environment is that at closure of the repository.

2. The source term at the boundary of the engineered barrier, i.e., boundary of the underground facility, is known.

3. The source term comprises scalar and vector quantities (heat, mass, and momentum).

4. The permeability of this zone is significantly different from that of the initial state and is time dependent.

5. The ground-water flow field is known at the initial time.

6. Thermophysical properties and geochemical constants are known functions of temperature.

7. Temperature and concentration gradients are significant at the boundary of the engineered barrier. At the boundary of the thermally undisturbed zone, the ambient geothermal and geochemical environment exists.

8. There are two time domains of significance: (1) containment and (2) controlled release.

Questions for Speakers and Panelists

1. What are the important transport processes in this spatial domain?

2. What are important couplings between these processes?

3. What criteria should be used to establish the relative importance of a transport process?

4. What are the major sources of uncertainty in geochemical, geomechanical, geothermal, and

hydrologic data that will potentially affect radionuclide transport?

5. What are the major sources of uncertainty in understanding and modelling radionuclide transport?

6. How does one bound radionuclide transport at this spatial scale? What modelling and experimental techniques should be used?

7. How can the validity of the above assumptions be tested?

ENGINEERED FACILITY AND WASTE PACKAGE

Definition

The waste package comprises the waste, primary container, additional containers and packing materials which are placed in the bored hole in the host rock.

Assumptions

1. Ground-water chemistry is known.
2. Packing and backfill material properties are known.
3. Overpack materials properties are known.
4. Thermal output per package and total thermal loading for the repository are known.
5. Corrosion kinetics of the primary and additional containers are known.
6. Leaching and dissolution kinetic of the waste is known.
7. A local flow field exists and is a known function of time and position.
8. The ground-water flow field is known at the initial time.
9. Thermophysical properties and geochemical constants are known functions of temperature.

Questions for Speakers and Panelists

1. How does early failure of one or more canisters affect subsequent canister failures?
2. What experimental tests are needed to determine the interactions between the waste package and the mined cavity and its engineered support system?
3. What tests are needed to assure that the waste and underground facility operate in the altered geologic environment according to design specifications?
4. What hydrothermal alterations in backing materials can be expected on the canister scale?

RES Workshop Waste Package Questions

1. What are the important processes which affect waste package containment and release? What are the important environmental parameters? What are the important couplings between the waste package processes and the environmental parameters? These questions should be addressed in terms of both the pre-closure and post-closure conditions.

2. What data are needed to support degradation process evaluations?

3. How do we develop an understanding and models for the above processes?

4. What are the major uncertainties in data and modeling of these processes?

5. How would one bound the above processes for data acquisition and for models?

6. How is the validity of the stated assumptions to be demonstrated?

WORKSHOP ON VALIDATION OF MATHEMATICAL MODELS FOR WASTE REPOSITORY PERFORMANCE ASSESSMENT - CONFIDENCE BUILDING THROUGH SYNTHESIS OF EXPERIMENTS AND CALCULATIONS

AB
Doc2
1/27/86

January 27 - 29, 1986

HOLIDAY INN HOTEL
8120 WISCONSIN AVENUE
BETHESDA, MARYLAND

PROGRAM

Sponsored by the

U.S. Nuclear Regulatory Commission

Office of Nuclear Regulatory Research

Organizers:

E. J. Bonano
Sandia National Laboratories
Tel: 505-844-5303

F. A. Kulacki
Colorado State University
Tel: 303-491-6603

J. D. Randall
U.S. Nuclear Regulatory Commission
Tel: 301-427-4633

- PROGRAM -

NATURAL BARRIERS - THERMALLY UNDISTURBED ZONE

Monday, January 27, 1986

Time	
8:30 - 8:45	INTRODUCTORY COMMENTS J. D. Randall, USNRC
8:45 - 9:05	LICENSING PERSPECTIVES ON MODELING S. Coplan, NRC
9:05 - 9:30	OVERVIEW OF WORKSHOP E. J. Bonano, SNLA
9:30 - 10:00	HYDROCOIN PROGRAM P. Davis, SNLA
10:00 - 10:15	INTRODUCTION OF SPEAKERS F. A. Kulacki, CSU
10:15 - 10:30	BREAK
10:30 - 11:00	TRANSPORT PHENOMENA Lynn Gelhar, MIT
11:00 - 11:30	HYDROLOGY S. P. Neuman, UAz
11:30 - 12:00	GEOCHEMISTRY M. Siegel, SNLA
12:00 - 12:30	DISCUSSION AND QUESTIONS FROM AUDIENCE Moderator: F. A. Kulacki, CSU
12:30 - 2:00	Lunch
2:00 - 3:45	PANEL DISCUSSION AND RESPONSE Moderator: G. Birchard, NRC Panelists: S. P. Neuman, Univ. of Arizona H. Wollenberg, LBL J. Daemen, Univ. of Arizona D. McLaughin, MIT D. Vogt, CorStar
3:45 - 4:00	BREAK
4:00 - 4:30	INTRAVAL PROGRAM K. Andersson, SKI
4:30 - 6:00	IDENTIFICATION OF NEEDED EXPERIMENTS AND VALIDATION PROCEDURES Moderator: F. A. Kulacki, CSU Participants: Keynote Speakers, Panelists, and Audience

- PROGRAM -

NATURAL BARRIERS - THERMALLY DISTURBED ZONE

Tuesday, January 28, 1986

Time	
8:30 - 8:45	INTRODUCTORY COMMENTS F. A. Kulacki, CSU
8:45 - 9:00	INTRODUCTION OF SPEAKERS E. J. Bonano, SNLA
9:00 - 9:30	HYDROLOGY (SATURATED MEDIA) P. A. Davis, SNLA
9:30 - 10:00	HYDROLOGY (UNSATURATED MEDIA) K. Preuss, LBL
10:00 - 10:15	BREAK
10:15 - 10:45	GEOCHEMISTRY D. Langmuir, Colorado School of Mines
10:45 - 11:15	GEOMECHANICS J. Noorishad, LBL
11:15 - 11:45	GEOMECHANICS C. Fairhurst, University of Minnesota
11:45 - 12:15	DISCUSSION AND QUESTIONS FROM AUDIENCE Moderator: E. J. Bonano, SNLA
12:15 - 1:30	Lunch
1:30 - 3:30	PANEL DISCUSSION AND RESPONSE Moderator: J. D. Randall, NRC Panelists: D. Evans, Univ. of Arizona C.-F. Tsang, LBL F. A. Kulacki, CSU K. Wahi, SNLA T. Nicholson, NRC D. Vogt, CorStar
3:30 - 3:45	BREAK
3:45 - 5:30	IDENTIFICATION OF NEEDED EXPERIMENTS AND VALIDATION PROCEDURES Moderator: E. J. Bonano, SNLA Participants: Keynote Speakers, Panelists, and Audience

- PROGRAM -

ENGINEERED BARRIERS - WASTE PACKAGE

Wednesday, January 29, 1986

Time	
8:30 - 8:45	INTRODUCTION J. D. Randall, NRC
8:45 - 9:00	OVERVIEW OF SESSION & INTRODUCTION OF SPEAKERS. J. D. Randall, NRC
9:00 - 9:30	BACKFILL & PACKING (COUPLED EFFECTS IN TRANSPORT. C. L. Carnahan, LBL
9:30 - 10:00	BACKFILL & PACKING (CHEMISTRY) C. Radke, LBL
10:00 - 10:15	BREAK
10:15 - 10:45	CORROSION A. Markworth, BCL
10:45 - 11:15	LEACHING & DISSOLUTION A. Markworth, BCL
11:15 - 11:45	DISCUSSION AND QUESTIONS FROM AUDIENCE Moderator: E. J. Bonano, SNLA
11:45 - 1:00	Lunch
1:00 - 3:00	PANEL DISCUSSION AND RESPONSE Moderator: K. Kim, NRC Panelists: J. Daemen, Univ. of Arizona M. Molecke, SNLA S. Nicolosi, BCL U. Bertocci, NBS H. Isaacs, Brookhaven M. McNeil, NRC D. Vogt, CorStar
3:00 - 3:15	BREAK
3:15 - 5:00	IDENTIFICATION OF NEEDED EXPERIMENTS AND VALIDATION PROCEDURES Moderator: F. A. Kulacki, CSU Participants: Keynote Speakers, Panelists, and Audience
5:00 - 5:15	CLOSING REMARKS F. A. Costanzi, NRC

AB
1/27/86
Doc 3

WORKSHOP ON

"VALIDATION OF MATHEMATICAL MODELS FOR WASTE REPOSITORY PERFORMANCE ASSESSMENT"

"CONFIDENCE BUILDING THROUGH SYNTHESIS OF EXPERIMENTS AND CALCULATIONS"

ORGANIZERS:
JOHN D. RANDALL, NRC
EVARISTO J. BONANO, SANDIA
FRANK A. KULACKI, COLORADO STATE UNIVERSITY

VALIDATION

ASSURANCE THAT MATHEMATICAL MODELS ARE ADEQUATE REPRESENTATIONS OF THE PROCESSES AND SYSTEMS WHICH THEY REPRESENT

MATHEMATICAL MODEL

PARTIAL OR ORDINARY DIFFERENTIAL EQUATION, INTEGRAL EQUATION, INTEGRO-DIFFERENTIAL EQUATION, ALGEBRAIC EQUATION

BOUNDARY CONDITIONS

INITIAL CONDITIONS

PROPERTIES

SYSTEM GEOMETRY

SETS OF THE ABOVE, POSSIBLY COUPLED TOGETHER

VALIDATION PROCESS

ITERATIVE PROCESS THROUGH WHICH EXISTING MODELS ARE USED TO IDENTIFY AND DESIGN NECESSARY LABORATORY AND FIELD EXPERIMENTS WHICH ARE THEN USED TO IMPROVE THE MODELS THEMSELVES

NRC OBJECTIVES FOR WORKSHOP

TO BRING TOGETHER EXPERIMENTALISTS AND MATHEMATICAL MODELERS TO BUILD A BASIS AND CONSENSUS FOR CONFIDENCE IN MODEL PREDICTIONS.

TO DEFINE CRITICAL EXPERIMENTS FOR TESTING MODELS AND THEIR SUPPORTING ASSUMPTIONS.

WHAT THE WORKSHOP IS AND IS NOT

IT IS A PLANNING MEETING FOR NRC'S HLW RESEARCH PROGRAM CONDUCTED BY NRC'S OFFICE OF NUCLEAR REGULATORY RESEARCH.

IT IS NOT A REVIEW OF THE NRC HLW RESEARCH PROGRAM.

IT IS NOT A PRELICENSING OR LICENSING POLICY MEETING. NO PRELICENSING OR LICENSING POLICY ISSUES WILL BE DISCUSSED IN THIS MEETING.

GROUND RULES

FOR SPEAKERS: PLEASE DO NOT SPEND MORE THAN YOUR ALLOTTED TIME ON PRESENTATIONS.

PLEASE RESTRICT YOUR PRESENTATIONS TO THE ISSUE OF **VALIDATION.**

FOR QUESTIONERS FROM THE AUDIENCE: PLEASE BE BRIEF IN YOUR QUESTIONS TO SPEAKERS DURING THEIR PRESENTATIONS. YOU MAY BRING UP LONGER QUESTIONS DURING THE SESSIONS ENTITLED "IDENTIFICATION OF NEEDED EXPERIMENTS AND VALIDATION PROCEDURES" EACH DAY.

PLEASE RESTRICT YOUR QUESTIONS TO THE ISSUE OF **VALIDATION.**

ORGANIZATION OF WORKSHOP

AVAILABILITY OF VIEWGRAPHS AND PAPERS

COPIES OF VIEWGRAPHS AND PAPERS PRESENTED AT THE WORKSHOP WILL BE MAILED TO THOSE WHO WANT THEM.

MAKE REQUESTS HERE AT THE WORKSHOP OR CONTACT

DR. JOHN D. RANDALL
MAIL STOP 1130SS
U. S. NUCLEAR REGULATORY COMMISSION
WASHINGTON, DC 20555
(301 OR FTS) 427-4633

IN YOUR REQUEST, PLEASE INDICATE THOSE PRESENTATIONS FOR WHICH YOU WISH TO HAVE COPIES OF VIEWGRAPHS AND/OR PAPERS.

THIS MATERIAL WILL ALSO BE INCLUDED IN THE FINAL REPORT OF THE WORKSHOP.