Sandia National Laboratories

Albuquerque, New Mexico 87185

May 15, 1990
Mr. David H. Tiktinsky
Office of Nuclear Material Safety
and Safeguards
Division of High-Level Waste Management
U.S. Nuclear Regulatory Commission
Mail Stop 6A-4
Washington, DC 20555

Dear Mr. Tiktinsky:

Enclosed is the April 1990 monthly report for FIN A1165. Also enclosed is a letter report discussing Quality Assurance criteria as applied to evaluating the application of HLW disposal system models. The contents of this letter report were originally a part of the Subtask 1.3e formal report; however, it was agreed that the material was too detailed for the formal report. We therefore agreed to incorporate the Quality Assurance criteria into a letter report and send it separately. D. Brosseau (ERCE) is the author of the report.

If you have any questions or comments, please feel free to contact me at (FTS) 844-5303, P. A. Davis at (FTS) 846-5421, or L. L. Price at (FTS) 844-6206.

Sincerely,

Evaristo J. Bonano, Supervisor
Waste Management Systems
Division 6416

EJB:6416

Enclosure

Copy to:

E. Davis
Office of the Director, NMSS
Attn: Program Support
Robert Browning, Director
Division of High-Level Waste Management
Seth Coplan
Division of High-Level Waste Management
Pauline Brooks
Division of High-Level Waste Management
John Randall
Division of Engineering

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6410	D. A. Dahlgren
6416	E. J. Bonano
6416	P. A. Davis
6416	L. L. Price
6416	K. K. Wahi
6416	D. A. Zimmerman
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SUMMARY SHEET

April 1990 Monthly Report for FIN A1165

Task	Activity	Costs
I	Licensing Methodology Assistance	$ 0K
II	Uncertainty Identification and Analysis	$ 0K
III	Probability Techniques	$ 0K
IV	Maintenance and Management of PA Codes	$ 0K
V	Technical Assistance for SCP Review	$ 0K
VI	Short Term Technical Assistance	$ 0K

PROGRAM:	Licensing-Methodology Assistance		FIN A1165 Task I
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/89 - 9/90
NMSS PROGRAM MANAGER:	P. Brooks	BUDGET AMOUNT:	$1K
CONTRACT PROGRAM MANAGER:	E. J. Bonano	FTS PHONE:	844-5303
PRINCIPAL INVESTIGATORS:	P. A. Davis	FTS PHONE:	846-5421
	L. L. Price	FTS PHONE:	844-6206

PROJECT OBJECTIVE

To assist in the overall development and integration of the licensing assessment methodology.

ACTIVITIES DURING APRIL 1990

Task I has been completed.

PROGRAM:	Identification and Analysis of Uncertainties	FIN A1165 Task II
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD: 10/89 - 9/90
NMSS PROGRAM MANAGER:	P. Brooks	BUDGET AMOUNT: $37K
CONTRACT PROGRAM MANAGER:	E. J. Bonano	FTS PHONE: 844-5303
PRINCIPAL INVESTIGATORS:	P. A. Davis L. L. Price	FTS PHONE: 846-5421 FTS PHONE: 844-6206

PROJECT OBJECTIVE

To identify, analyze, and recommend generic methodologies for treating uncertainties associated with performance assessments of HLW repositories.

ACTIVITIES DURING APRIL 1990

Subtask 2.1

I. Recommended techniques for assessing compliance with the EPA's HLW repository containment requirement (40 CFR 191.13)

A draft of this report was sent to the NRC on January 16, 1990. We received the NRC's comments on March 22, 1990. Internal reviews of the report have been completed, and we are in the process of addressing the NRC's comments.

Subtask 2.2/2.6c

I. Identification, evaluation, quantification, and reduction of uncertainty in HLW repository performance assessments.

A draft of this report was sent to the NRC on April 2, 1990. We are waiting for NRC comments. The report is currently being reviewed internally at SNL.

Subtask 2.3

I. Elicitation and use of expert judgement in dealing with uncertainty in HLW repository performance assessments.

The final camera-ready original of this report was sent to the NRC for publication on April 23, 1990. In addition, a copy of this original was sent to Pauline Brooks on April 23, 1990. SNL's obligation with respect to Subtask 2.3 has been fulfilled.

Subtask 2.4

I. Methods for analyzing uncertainty in HLW repository performance assessment models.

A draft of this report was sent to the NRC on February 7, 1990. We are waiting for NRC comments. Internal reviews of the report have been completed.

Subtask 2.5

Completed

Subtask 2.6

I. Recommended methodologies for the analysis of data and parameter uncertainty in HLW repository performance assessment.

Completed

IV. Uncertainty and sensitivity analysis in ground-water flow modeling.

A draft of this report was sent to the NRC on February 27, 1990. We are currently waiting for NRC comments. Internal reviews of the report have been completed.

PROGRAM:	Probability Techniques		FIN A1165 Task III
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/89 - 9/90
NMSS PROGRAM MANAGER:	P. Brooks	BUDGET AMOUNT:	$16K
CONTRACT PROGRAM MANAGER:	E. J. Bonano	FTS PHONE:	844-5303
PRINCIPAL INVESTIGATORS:	P. A. Davis	FTS PHONE:	846-5421
	L. L. Price	FTS PHONE:	844-6206

PROJECT OBJECTIVE

To identify techniques for assigning probabilities to geologic processes and events.

ACTIVITIES DURING APRIL 1990

Subtask 3.2

I. Recommended techniques for estimating probabilities of events and processes affecting the performance of geologic repositories: assessing compliance with the EPA's containment requirements (40 CFR 191.13).

A draft of this report was sent to the NRC on February 21, 1990. We are currently waiting for NRC comments and are having the report reviewed.

PROGRAM: Short-Term Technical Assistance

FIN A1165
Task VI

BUDGET AMOUNT: $3K

PROGRAM OBJECTIVE

To provide, on short notice, general technical assistance on HLW matters related to Tasks 1 through 5 that would not be provided in the normal course of the work in these tasks.

ACTIVITIES DURING APRIL 1990

No activity this month

SCHEDULE OF MILESTONES AND DELIVERABLES

SUBTASK NUMBER	DELIVERABLE TITLE	DRAFT DUE	FINAL DUE	STATUS
1.1	Components of an Overall Performance Assessment Methodology	Submitted Dec. 1, 1988	Submitted Jan. 31, 1990	Completed
1.3e	Technical Basis for NRC Review of HLW Repository Modeling	Submitted June 14, 1989	Submitted Feb. 8, 1990	Completed
2.1	Techniques for Assessing Compliance with the EPA's HLW Repository Containment Requirement	Submitted Jan. 16, 1990	No due date.	Addressing NRC comments.
2.2/2.6c	Uncertainties Associated with Performance Assessment of High-level Radioactive Waste Repositories: A Summary Report	Submitted April 2, 1990	No due date.	Waiting for NRC comments.
2.3	Elicitation and Use of Expert Judgment in Performance Assessments for HLW Repositories	Submitted July 26, 1990	Submitted Apr. 23, 1990	Completed.
2.4a	Guidelines for Judging the Validity of Models for Performance Assessment of HLW Repositories	Submitted Feb. 7, 1990	No due date.	Waiting for NRC comments.

2.5	Risk Methodology for Geologic Disposal of Radioactive Waste: Scenario Selection Procedure	Submitted June 27, 1989	Submitted Mar. 26, 1990	Completed.
2.6a	A Review of Techniques for Propagating Data and Parameter Uncertainty in High-Level Radioactive Waste Repository Performance Assessment Models	Submitted May 31, 1989	Submitted Feb. 15, 1990	Completed.
2.6d	A Comparison of Parameter Estimation and Sensitivity Analysis Techniques for Ground-Water Flow Models and Their Impact on the Uncertainty in Model Performance Predictions	Submitted Feb. 27, 1990	No due date.	Waiting for NRC comments.
3.2	Techniques for Determining Probabilities of Events and Processes Affecting the Performance of Geologic Repositories: Volume II --Suggested Approaches	Submitted Feb. 21, 1990	No due date.	Waiting for NRC comments.

SUBTASK 1.3(E) LETTER REPORT
RECOMMENDED APPROACHES FOR EVALUATING THE APPLICATION OF HLW DISPOSAL SYSTEM MODELS

1.0 Background

In order to license a HLW repository, the DOE has been given the responsibility to carry out a program of site characterization and performance analyses to demonstrate "reasonable assurance" that burial of nuclear wastes will pose no undue risk to the public health and safety. It is expected that mathematical and numerical analyses based upon models representative of repository design, natural processes, and repository response to those environmental processes will be performed by the DOE. It will be the responsibility of the NRC to evaluate these DOE models to ensure that they are based on sound physical and mathematical principles, and that they are correctly applied.

A license application from the DOE for a HLW repository must consist of, in addition to other data and information, a Safety Analysis Report which describes the repository site and assesses those features that might adversely affect repository performance. The NRC regulations, 10 CFR Part 60.21(c)(1), specify the description and analyses required in the SAR. Paragraph (ii)(A) requires "An analysis of the geology, geophysics, hydrogeology, geochemistry, climatology, and meteorology of the site." Paragraph (ii)(B) requires "Analyses to determine the degree to which each of the favorable and potentially adverse conditions, if present, has been characterized, and the extent to which it contributes to or detracts from isolation..." Paragraph (ii)(C) requires, in part, "An evaluation of the performance of the proposed geologic repository for the period after permanent closure..." Finally, paragraph (ii)(D) specifies assessment of "The effectiveness of engineered and natural barriers, including barriers that may not be themselves a part of the geologic repository operations area, against the release of radioactive material to the environment."

For these analyses, the DOE must provide in the SAR (per 10 CFR 60.21(c)(1)(ii)(F)):

> "An explanation of measures used to support the models used to perform the assessments required in paragraphs (A) through (D). Analyses and models that will be used to predict future conditions and changes in the geologic setting shall be supported by using an appropriate combination of such methods as field tests, in situ tests, laboratory tests which are representative of field conditions, monitoring data, and natural analog studies."

To accomplish the above, the DOE must include in its program the development and implementation of models and computer codes, plus obtain and use appropriate input data, adequate to perform such analyses. It will be DOE's responsibility to ensure the adequacy of analyses and the quality of all data used. The burden of proof regarding compliance with regulatory criteria lies with the DOE. The role of the NRC will be to review the license application, and specifically the adequacy of models and codes used, for adherence to regulatory requirements and determination that authorization to design and construct a HLW repository has been justified. It will not be the role of NRC to develop models and codes for the DOE, to acquire input data, nor to provide analyses supportive of the DOE analytical efforts. However, the NRC may independently use, and develop as required, codes to evaluate the DOE submittals and analyses.

2.0 Objective

The objective of this report is to provide recommended approaches and the technical basis for the NRC in their evaluation of the DOE modeling efforts. Approaches will be provided for peer reviews of analyses performed by the DOE, plus independent evaluations performed by NRC staff to assess the DOE modeling approach. Review criteria are established for evaluating model assumptions and validity, data representativeness, model and data uncertainty, and appropriateness of model application to the analyses being performed.

The NRC will need to selectively review the various areas of analyses, depending upon time constraints, resources, staff availability, and uncertainties involved. The level of review will vary depending on NRC policy and the degree of risk involved. Because of the many analyses involved over significant periods of time, requiring numerous areas of expertise, a review strategy will be used to determine the appropriate levels of detail necessary in the licensing reviews. The following section provides a comprehensive discussion of the quality assurance aspects of the evaluations of HLW disposal system modeling applications.

3.0 QA Requirements for Codes

One important aspect in the overall analytical program used by the DOE, and evaluated by the NRC, is the proper implementation of quality assurance requirements. Subpart G of 10 CFR Part 60 calls for quality assurance programs modeled after the provisions of 10 CFR Part 50, Appendix B for all activities related to and "important to safety" and "important to waste isolation." NUREG-1318 provides the position that "those activities related to the actual performance assessments...should be controlled under a Subpart G QA program." Because modeling and numerical analysis using computer codes to assess performance are clearly activities "related to the actual performance assessments", it follows that quality assurance provisions must be implemented when conducting such analyses.

Performance analyses will be conducted for natural processes and repository response which will occur over a regulatory period of many thousands of years. Since the design and operation of a HLW repository has never been attempted before and not all of the processes involved are well understood, it will be difficult to show, without significant uncertainties, that all of the performance objectives outlined in 10 CFR Part 60 can be met. Therefore, the regulations state that "...what is required is reasonable assurance, making allowance for the time period, hazards, and uncertainties involved, that the outcome will be in conformance with those objectives and criteria" (10 CFR Part 60.101(a)(2)). Absolute proof and correctness of analytical models cannot be provided; however, use of expert judgment, tests, field data, monitoring data, and natural analog studies to "validate" and calibrate models should provide the "reasonable assurance" required, if properly documented and supported. Quality Assurance will ensure the appropriate levels of documentation are provided.

3.1 Computer Codes, Data, and Results

In studies to date sponsored by the NRC, DOE, and others, many analytical models and computer codes have already been developed to address HLW repository design and performance assessment. New computer codes are currently being developed as analyses identify the need for new models. The DOE will be using many currently operational codes, plus new codes, in their efforts to provide a licensing basis for the HLW repository. In turn, the NRC will either review those analyses, perhaps by verifying the results using the same codes, or will use other codes to assess the validity of the DOE results.

The parameters and data used to construct the models and run the codes must be determined based on preliminary studies and knowledge gained from the site characterization studies. Data will be collected from scientific investigations and existing data bases and used in the development, verification, validation, and calibration activities associated with the codes. Experience with the codes will in turn identify additional or more appropriate data needs. This interactive process will be necessary to develop and improve the models towards meeting the goal of reasonable assurance. Uncertainty and sensitivity analyses will be required to assess the quality and adequacy of the data used with and the results obtained from the models.

The following sections address the QA requirements with respect to models, computer codes, and data.

3.2 Computer Code and Model QA

Conceptual models are the general understanding of the designer or scientist for a given system under study. A conceptual model is, at best, a limited representation of the real system which ideally captures all of the important attributes of the system required to understanding system response for the range of parameters and system states of interest. When combined with data and properly coded, the model can be compared with observed behavior to predict some performance assessment measure of interest. The mathematical or numerical codes are the quantitative means for solving the equations developed to simulate the model processes being investigated.

Quality assurance, as applied to computer software, can be defined as a planned and systematic pattern of all actions necessary to provide adequate confidence that the models and computer software conforms to established technical requirements. This definition of software quality assurance can be interpreted to mean a plan by which computer codes, data sets, operating instructions, and interfaces are developed and maintained in a fashion that assures the reliability of the results within the limitations of the mathematical principles, data availability, and hardware. Quality assurance provisions should apply to all phases of efforts devoted to conceptual modeling, code design, code verification and validation, code calibration, code baselining, code maintenance, and code documentation and usage. A few definitions are in order.

Verification is a demonstration that a code solves the mathematical equations it was designed to solve, correctly. This is accomplished by comparison to analytical solutions, or similar results of another verified code (benchmarking).

Validation is the process which demonstrates that the mathematical model embodied in the software is an acceptable representation of the process or system for which it is intended, (NQA-3 Draft, 1988). This is an ongoing process which builds confidence in the code and shows regions of applicability. Validation is usually accomplished by comparison of results with physical data.

Benchmarking is use of a set of problems which have been solved by other codes designed to solve the same basic equations.

Model calibration is the process in which the model and its input parameters (and their spatial and/or temporal distributions) and boundary conditions are adjusted or fine-tuned (taking care not to exceed reasonable limits, as determined from observed data and system understanding) to bring predicted performance into relative agreement with the real system. Calibrated models are then used in uncertainty and sensitivity studies done to gain insight regarding the dependence of specific predicted system responses to varying values for given parameters.

Baselining is establishment of a point in the software lifecycle where identified work is completed and reviewed and all documentation to that point has been prepared. A baselined code is usually placed into configuration management.

Configuration management is a system for orderly control of software and all subsequent changes to that software and its associated documentation.

The ability of the DOE to demonstrate quality in performance assessment efforts depends on DOE having an adequate quality assurance program in place during the planning and conduct of all analyses and data acquisition for prelicensing assessment. As stated earlier, Subpart G of 10 CFR Part 60 requires a QA program in accordance with the provisions of 10 CFR Part 50, Appendix B. The QA program should be presented in sufficient detail to allow the NRC to make an independent evaluation of the technical adequacy and implementation of appropriate analyses to support a license application. Unfortunately, the Appendix B QA criteria were originally developed for the design, construction, and operation of nuclear power plants. Some of the requirements of Appendix B do not specifically apply to nuclear waste repositories and the analytical performance assessment efforts associated with them. For example, criteria such as Identification and Control of Materials, Parts and Components; Control of Special Processes; Inspection; Test Control; Control of Measuring and Test Equipment; and Handling, Storage and Shipping are all clearly applicable to power plant hardware-oriented activities and do not specifically apply to software and analysis. Additionally, the unique nature of HLW repositories will require additional QA guidance not provided in Appendix B. This would involve unique controls for items such as coding standards, configuration management, and verification activities.

Current efforts are underway at the NRC and within the ANSI/ASME committees on Nuclear Quality Assurance (NQA) to develop additional guidance specific to HLW disposal activities. The final position on HLW QA will be based on the basic applicable criteria of Appendix B, recent experience with DOE and NRC HLW activities, the general guidance provided in NQA-1, and new guidance being developed for the proposed NQA-3, "Quality Assurance Program Requirements for the Collection of Scientific and Technical Information for Site Characterization of High-Level Nuclear Waste Repositories." Important lessons learned from reactor programs, differences in terminology, and the special needs with respect to performance assessment, scientific investigations, and acquiring and using data in analyses, need to be addressed in QA provisions for HLW activities. The DOE will be conducting scientific investigations to produce data on the natural conditions existing at the site, and using this data with existing data in performance assessment to determine if the site can meet the performance objectives of 10 CFR Part 60. The applicable requirements of Appendix B and the DOE QA Plans need to be supplemented to address these areas. Currently, for instance, Appendix H of the DOE NNWSI/88-9 "Nevada Nuclear Waste Storage Investigations Project Quality Assurance Plan" has been accepted by the NRC staff for implementation of software QA provisions.

Quality assurance programs for computer models and codes are needed to spell out the requirements unique to code design and usage. Software QA can be applied over the entire "lifecycle" of software development, testing, use, and maintenance. Since the HLW disposal program analytical efforts will undoubtedly involve use of both existing and new codes, plus modifications to existing codes, it will be important for software QA plans to address the quality aspects of the various software phases. Guidance for the development of software QA plans is provided in ANSI/IEEE Standard 730-1984, "IEEE Standard for Software Quality Assurance Plans." Additional guidance is provided in NUREG/CR-4640, "Handbook of Software Quality Assurance Techniques Applicable to the Nuclear Industry." These documents outline approaches to software QA for the entire lifecycle and include items such as the following:

a. Purpose
b. Reference documents
c. Management
d. Documentation
e. Standards, practices and conventions
f. Reviews and audits
g. Configuration management
h. Problem reporting and corrective action
i. Tools, techniques and methodologies
j. Code control
k. Media control
l. Supplier control
m. Records collection, maintenance and retention

All or any part of the above "requirements" may apply, depending on the nature of the software. The following sections provide discussions on various aspects of software QA relative to HLW disposal programs.

1. Code Development

Ideally, the vast majority of quality assurance efforts for software should be focused on the developmental phases. Simply maintaining existing code and "inspecting in quality" is not enough. It is unreasonable to expect quality assurance at the "back end" to compensate for a disregard for quality in the developmental period.

All new codes developed by the DOE or it's contractors should include provisions for quality assurance as outlined in IEEE 730. Quality must be built into software during its development. This would include such things as documented concept and requirements definition, preliminary and detailed design descriptions, verification and validation plans, coding standards, testing, and reviews throughout the process. The goal is to establish the "correctness" and adequacy of the model and code to solve the problems they were intended for. As a minimum, all modeling efforts should be traceable, retrievable, and documented to meet the approval of the NRC.

2. Operational Codes

Existing codes or operational codes, as opposed to codes under development, will be used for many of the analyses required for DOE to demonstrate performance. For these cases, quality assurance may focus on the "housekeeping" tasks of configuration management and error detection/correction. However, a review of the quality provisions applied during development of the code must be made. The prior existence and use of the code does not simply imply it is an adequate code. The review should consider the same criteria as is recommended for a newly developed code. Unfortunately, some codes have been developed without benefit of a full, if any, quality assurance program. In these cases, a critical assessment of the code to qualify it for use in a particular application must be made by the DOE. This qualification must be based on the ability of the software to provide acceptable results for the problems and to show compliance with the technical and quality requirements. This process may include verification and validation activities, establishment of a documented software baseline, initiation of configuration management, and full documentation to support the software for use and review. All of these qualification activities also apply to major modifications to existing codes to adapt them to a particular class of analyses. A program including written policies and procedures should be in place to ensure that these activities are conducted in a consistent and systematic manner.

3. Verification and Validation

Verification and validation activities must be planned, conducted in accordance with procedures, and documented. It is important to note that these activities must be viewed as an ongoing process. As more information about site geology and hydrology becomes available, and additional understanding of the physical processes is gained, models and the data used with the models will be continually refined and updated, until model confirmation is considered complete. Since "complete" validation is an ideal, not to be fully realized for the complex models needed for repository performance assessment, a point must be reached by systematic methods to demonstrate adherence to the principle of "reasonable assurance".

Verification is relatively straight-forward and can be accomplished using appropriate methods such as inspection, peer review, testing, analysis, or demonstration. Adequate planning, reviews and documentation of the process are key. Verification is really associated with the development process, and is difficult to "backfit", especially for large, complex codes that have been years in development. Verification activities must always relate back to the original objectives and requirements of the code.

If those requirements can be verified in all later phases of development, then there is good assurance that the code does what it was intended to do. It is very important to have well-defined requirements that can be implemented and that are testable. Verification proceeds in steps throughout the software lifecycle and demonstrates cohesion between steps and the traceability of the code. The model itself, as well as the mathematical and numerical representations, must be verified. Use of structured techniques and modular design will help simplify the verification process. With adequate documentation of this process, re-verification of later changes and modifications to the software can be accomplished easily. The amount of verification necessary is a judgment call that the DOE must make based on the complexity and criticality of the particular code.

Complete validation of complex codes used for repository analysis will never be achieved. Validation must be tied into the original requirements specification and the problem at hand. Validation is accomplished by comparing software results against verified and traceable data obtained from laboratory or field experiments, or in situ testing. When data are lacking, alternate approaches used to evaluate the validity of models must be documented. Use of peer reviews and expert judgment will be one approach used in attempting to validate computer models. It will be important to ensure that the model is adequate for its intended use.

4. Configuration Management

A configuration management system must be in place during development of mathematical models and computer code. For the "finished" software, configuration management must establish identification of a particular baseline and control changes to the software. All code versions and revisions must be uniquely controlled, with the data and results used for that given configuration, along with verification and benchmark problems associated with that particular version of the code. Configuration management must be formally controlled and documented. This is sometimes achieved by a separate "operational" software QA plan which spells out all of the requirements unique to this aspect of software quality (for example, reference can be made to NUREG/CR-4369, "Quality Assurance (QA) Plan for Computer Software Supporting the U.S. Nuclear Regulatory Commission's High-Level Waste Management Program"). Configuration management should address means to control access to software codes to prevent unauthorized changes and modifications. Physical media used for storage and documentation should be controlled and protected from loss or unauthorized use and to ensure retrievability. Procedures must be in place to control and document the methods used to identify, control, record, update, track, store, and document all changes to the software.

Procedural and documentational means must be developed to control the reporting and disposition of problems identified during use of the code. Each problem should be separately identified, documented and tracked via systematic means. Following identification of root causes, potential solutions and changes to the code must be analyzed. Proposed changes should be reviewed and subjected to verification testing to prevent new problems from surfacing in the process of solving the original problem. As changes are implemented, they should be entered into the configuration management system, either singly or as a group of changes which result in issuance of a new code version or update. Effective communication between code users and the code sponsor/developer must be a part of this process. Means must be provided for assessment of the effects of code changes on previous calculations performed with the prior "defective" code.

5. Documentation

NUREG-0856, "Final Technical Position on Documentation of Computer Codes for High-Level Waste Management," (NRC, 1983), provides the best guidance for establishing and assessing adequate code documentation. Recommended documentation falls into five categories, including:

a. Software summary
b. Description of mathematical models and numerical methods
c. User's manual
d. Code assessment and support
e. Continuing documentation and code listings

This document should be consulted for specific guidance. It should be used as the criteria against which DOE documentation implementation is assessed.

6. Analysis Documentation: Code, Data, Results

Simply documenting the validity of a particular model and associated computer code for an analysis application will not be sufficient to support the license application for a HLW repository. The codes, together with all input parameters and data, and the model results must all be documented in a defendable, traceable, and retrievable manner. Enough detail must be presented to allow the code and data to be independently run by the NRC. The calibration of code parameters, input data, and predictions will be important as an integral part of model validation which demonstrates the adequacy of the model. As new data and insights are gained during the course of site characterization and other scientific investigations, re-analysis may be required utilizing data which may better represent the physical systems. This entire process, likely to involve numerous organizations over many years, must be controlled and documented in a systematic manner. Thus, effective quality programs and management oversight are imperative. Use of both quality assurance procedures and technical procedures subject to close scrutiny in technical reviews, peer reviews, and periodic independent assessments will be mandatory.

3.3 Data Quality Assurance

Having data that is as accurate and representative as possible in performance assessments is paramount. The information and data which is collected and analyzed will be used by the DOE as part of the technical basis to support a license application to the NRC for a HLW repository. By association, the QA program requirements which apply to computer codes also will apply to data acquisition and use in modeling efforts. In addition, the regulations specifically require quality programs during site characterization. In 10 CFR Part 60.17(a)(1), the contents of the site characterization plan must contain, in the general plan:

> "A description of such area, including information on quality assurance programs that have been applied to the collection, recording, and retention of information used in preparing such description."

Also, the general plan will include a description of site characterization activities, including (10 CFR Part 60.17 (a)(2)(v)):

> "Plans to apply quality assurance to data collection, recording, and retention."

As stated earlier, the quality assurance provisions must be established according to the 18 criteria of Appendix B of 10 CFR Part 50. The program must address the plans and detailed procedures for data collection, analysis, manipulation, recording, and retention. Data information needs are established by preliminary analyses based on performance objectives and site specific conditions. Once data needs are determined and test plans/procedures are established (all of which is an ongoing process), then provisions must be made for data selection and collection, data interpretation, and data manipulation.

1. Data Selection and Collection

Numerous types and quantities of data for use in repository models will be collected over long periods of time from numerous sources. Both new and preexisting data will need to be acquired. Due to the large area of data coverage required and, in some cases, the long time periods for which data is needed (precipitation, for instance), use of and evaluation of historical data will constitute a large percentage of the data required. Plans and procedures must address the data needs and all potential data sources. Provisions must be included for verification of data. Verification in this case means that data are accurate and of sufficient precision. Other characteristics of quality data which may require evaluation are that data should be valid, defensible, comparable, complete and representative of a population or parameter.

The data collected must also be linked with the needs of the models for which it will be used. Attention must be paid to the compatibility of the data and its form with the input requirements of the computer codes. The sophistication of the code should also be factored into the level of effort needed for acquiring the data. Simple computer modeling which may be used for performance assessments may not require extensive efforts to acquire data which is highly accurate and difficult to obtain.

Some characteristics which should be included in quality assurance programs associated with the acquisition of data include:

a. The identification of and intended use for the data should be spelled out in planning documents, as well as the evaluations mentioned above.

b. Written plans and procedures, with peer review.

c. Use of qualified test personnel and equipment.

d. Adequate sampling provisions, including sample identification; traceability; handling, storage and transport; and documentation and records.

e. Sample test and results analysis procedures.

f. Data transfer and data reduction procedures.

g. Control provisions for erroneous or inadequate data.

h. Data identification and traceability to tests and sources.

i. Records requirements, retention, storage, access control, retrievability procedures and facilities.

j. Use and documentation of peer reviews of all phases of scientific investigations for data acquisition, including requirements and planning, procedure preparation, conduct of testing and experiments, and analysis of results.

Preexisting data should be evaluated in accordance with written procedures and its qualification for use documented. Factors to be considered should include:

a. Review of the relevant qualifications of personnel or organizations who originally generated the data.

b. Assessment of the adequacy of the equipment and procedures used to collect the data.

c. Consideration of environmental conditions during data collection.

d. Analysis of measurement control and the quality and reliability of the measurement instrumentation and procedures used, including calibration provisions.

e. An overall assessment of data quality using a combination of qualification methods which might include peer reviews, comparison with corroborating data, confirmatory testing, checks for internal consistency and reasonableness of data sets, evaluation of extrapolated data, comparison of data with results of model simulations, and demonstration that data were collected under a QA program equivalent to that used for new data.

2. Data Interpretation

Interpretation of data really includes validation of data which, in this context, means demonstrating that data correctly represents the process or system and are being correctly applied. The analysis of data validity must be documented following a systematic methodology. Evaluations must be made for those instances involving missing data or partial data sets, due perhaps to problems encountered during the original period of data acquisition. Extrapolation, interpolation, and regionalization of data must be closely evaluated to ensure these interpretations are based on sound judgment and techniques. In some instances, conservatism of data would need to be assessed to ensure it is still representative of the full field of data and the system or process analyses it will be used in conjunction with.

A key element related to and responsible for the assignment of conservatism to data is data uncertainty. It is important in assessments of or the interpretation of data that uncertainty be evaluated and factored into models which will use the data. Uncertainties must be identified, quantified, and reduced where possible. Sensitivity analyses may be used to evaluate the significance of data uncertainties with respect to the overall uncertainty in repository system performance. Potential sources of uncertainty related to data include:

a. Measurement instrument error, or operator error.

b. Error in the interpretation or translation of the field measurements into a value for the parameter of interest in the associated model.

c. Extrapolation errors resulting from the process of developing an estimate for the spatial and/or temporal distribution of parameters from point measurements of the parameters.

All assessments of data uncertainty should be controlled and documented completely using procedures and methods established by quality program provisions.

3. Data Manipulation

Manipulation of data is needed to adapt the data to the requirements of performance assessment computer models and to evaluate the effects of changes to input data. It is imperative that quality provisions for data manipulation are spelled out in planning documents and in QA implementing and technical procedures. Model and code documentation must address the data file requirements and the techniques used for inputting data. This might include descriptions of how files are read and written, data input field and data base structure, retention and/or reinitialization of input parameters, and default settings.

The methods and procedures used to "calibrate" models should be prepared and actual calibration efforts documented. Spatial and temporal distributions of data must be defined and assessed, and boundary conditions established for the ranges of calibration under study. The data and input used in calibration and model development efforts should be different from measured field values which will be compared to model predictions. The results of calibration efforts and justifications for when calibration is considered complete must be thoroughly documented.

Calibrated models will undergo sensitivity analyses which will involve adjustment of data and input parameters to study the effects on model behavior and predictions. Sensitivity analyses will be used to evaluate such things as missing or incomplete data, data uncertainty, process modeling uncertainty, and temporal uncertainties. All sensitivity analyses need to be planned and documented and should include system definition, identification of parameter ranges over which the system is to be investigated, and the characteristics of the system which are to be observed.

3.4 Peer Review and Independent Evaluation - Quality Factors

To evaluate the validity and appropriate application of DOE modeling efforts, the NRC will conduct both peer reviews and independent evaluations of submittals from the DOE for support of HLW repository licensing. The former will be used for those analyses which are relatively straight forward and for which known and familiar, verified and validated computer codes are used. Review of the models themselves and validity and use of data will be conducted without resorting to separate computer models. The latter will be used for analyses using newly developed codes which are not well known and for those cases that the NRC does not agree with or suspects the quality or technical content of the DOE submittals. These evaluations will require modeling efforts and analyses to be conducted by NRC staff to compare with DOE results. Model and data selection, plus analytical efforts, will need to be responsive to the requirements stated in this document.

The strategy for NRC review of HLW performance assessment using numerical models and computer codes has been addressed in the "Revised Modeling Strategy Document for HLW Performance Assessment," (NRC, 1984), which is scheduled for revision. The development, evaluation, and application of models to be used independently by the NRC must follow the guidance provided in this document. It is the intent of this section to discuss briefly the QA aspects required to successfully perform the reviews and evaluations the NRC may conduct.

1. Peer Review

One of the most important aspects of any review is identification of the applicable review criteria to be used for conduct of the reviews. These will be based on the requirements of the regulations and guidance provided in documents such as this one. For peer reviews, the objectives should fall along the lines of reviewing the completeness and accuracy of (a) the models, (b) model inputs and data quality, (c) results, (d) sensitivity and uncertainty determinations, and (e) assessment of alternative analyses and interpretations. The level of detail in such reviews is subject to the technical judgment of NRC staff, available resources, and timing considerations. This determination of review level is, in itself, an important aspect of the peer review planning process. Analysis of uncertainties will play an important part in deciding how much detail is required in a given peer review.

One source of guidance for the peer review process is NUREG-1297, "Peer Review for High-Level Nuclear Waste Repositories," (NRC, 1988). All peer reviews should be planned, with key consideration being given to the qualifications and independence of the review group and individuals. The reviewers should be selected to span the technical issues involved. Technical qualifications should be documented, with skills at least equivalent to that needed to perform the work under review. Peer reviewers should have no direct involvement as a participant, supervisor, technical reviewer, or advisor in the work being reviewed. Where technical expertise is not available or where strict independence is not met, a documented rationale should be provided for the review team selected. Procedures for peer review must be developed and the planning and conduct of peer reviews documented. Peer reviewers should document their findings, addressing the suitability of the work being reviewed for its intended