Designation: C 1174 – 07

Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste[1]

This standard is issued under the fixed designation C 1174; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ϵ) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice describes test methods and data analyses used to develop models for the prediction of the long-term behavior of materials, such as engineered barrier system (EBS) materials and waste forms, used in the geologic disposal of spent nuclear fuel (SNF) and other high-level nuclear waste in a geologic repository. The alteration behavior of waste form and EBS materials is important because it affects the retention of radionuclides by the disposal system. The waste form and EBS materials provide a barrier to release either directly (as in the case of waste forms in which the radionuclides are initially immobilized), or indirectly (as in the case of containment materials that restrict the ingress of groundwater or the egress of radionuclides that are released as the waste forms and EBS materials degrade).

1.1.1 Steps involved in making such predictions include problem definition, testing, modeling, and model confirmation.

1.1.2 The predictions are based on models derived from theoretical considerations, expert judgment, interpretation of data obtained from tests, and appropriate analogs. 1.1.3 For the purpose of this practice, tests

1.1.3 For the purpose of this practice, tests are categorized according to the information they provide and how it is used for model development and use. These tests may include but are not limited to the following:

1.1.3.1 Attribute tests to measure intrinsic materials properties,

1.1.3.2 Characterization tests to measure the effects of material and environmental variables on behavior,

1.1.3.3 Accelerated tests to accelerate alteration and determine important mechanisms and processes that can affect the performance of waste form and EBS materials,

1.1.3.4 Service condition tests to confirm the appropriateness of the model and variables for anticipated disposal conditions,

1.1.3.5 Confirmation tests to verify the predictive capacity of the model, and

1.1.3.6 Tests or analyses performed with analog materials to identify important mechanisms, verify the appropriateness of an accelerated test method, and to confirm long-term model predictions.

1.2 The purpose of this practice is to provide methods for developing models that can be used for the prediction of materials behavior over the long periods of time pertinent to the service life of a geologic repository as part of the basis for performance assessment of the repository.

1.3 This practice also addresses uncertainties in materials behavior models and their impact on the confidence in the performance assessment.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory requirements prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:* [2]

C 1285 Test Methods for Determining Chemical Durability of Nuclear, Hazardous, and Mixed Waste Glasses and Multiphase Glass Ceramics: The Product Consistency Test (PCT)

E 177 Practice for Use of the Terms Precision and Bias in ASTM Test Methods

E 178 Practice for Dealing With Outlying Observations

E 583 Practice for Systematizing the Development of (ASTM) Voluntary Consensus Standards for the Solution of Nuclear and Other Complex Problems[3]

2.2 *ANSI Standard:*[4]

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[1] This practice is under the jurisdiction of ASTM Committee C26 on Nuclear Fuel Cycle and is the direct responsibility of Subcommittee C26.13 on Spent Fuel and High Level Waste.

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[2] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

[3] Withdrawn.

[4] Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, http://www.ansi.org.

ANSI/ASME NQA-1 Quality Assurance Program Requirements for Nuclear Facility Applications

2.3 *U.S. Government Documents:*

DOE/RW-0333P, Assurance Requirements and Description, USDOE OCRWM, latest revision

Code of Federal Regulations, Title 10, Part 60, Disposal of High-Level Radioactive Wastes in Geologic Repositories, U.S. Nuclear Regulatory Commission, January 1997[5]

Code of Federal Regulations, Title 10, Part 63, Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada, U.S. Nuclear Regulatory Commission, latest revision[5]

Code of Federal Regulations Title 40, Part 191, Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes, July 2002[5]

Public Law 97-425, Nuclear Waste Policy Act of 1982, as amended

NUREG–0856, Final Technical Position on Documentation of Computer Codes for High-Level Waste Management (1983)[6]

3. Terminology

3.1 *General Definitions*:

3.1.1 Terminology used in this practice is per existing ASTM definitions, or as understood per the common English dictionary definitions, except as described below.

3.2 *Regulatory and Other Published Definitions*—Definitions of the particular terms below are based on the referenced Code of Federal Regulations, 10 CFR 63 and/or 10 CFR Part 60 which is pertinent to this standard and is under jurisdiction of the Nuclear Regulatory Commission (NRC). If precise regulatory definitions are needed, the user should consult the appropriate governing reference.

3.2.1 *disposal*—the emplacement in a repository of high-level radioactive waste, spent nuclear fuel, or other highly radioactive material with no foreseeable intent of recovery, whether or not such emplacement permits the recovery of such waste.

3.2.2 *engineered barrier system (EBS)*—the waste packages and the underground facility, which means the underground structure including openings and backfill materials.

3.2.3 *geologic repository*—a system which is intended to be used for, or may be used for, the disposal of radioactive wastes in excavated geologic media. A geologic repository includes the geologic repository operations area, and the portion of the geologic setting that provides isolation of the radioactive waste.

3.2.4 *important to safety*—refers to those engineered features of the geologic repository operations area whose function is: *(1)* To provide reasonable assurance that high level waste can be received, handled, packaged, stored, emplaced, and retrieved without exceeding regulatory requirements for Category 1 design basis events; or *(2)* To prevent or mitigate Category 2 design basis events that could result in doses equal to or greater than the regulatory values to any individual located on or beyond any point on the boundary of the site.

3.2.5 *important to waste isolation*—refers to those engineered and natural barriers whose function is to provide reasonable assurance that high-level waste can be disposed without exceeding the regulatory requirements.

3.2.6 *high-level radioactive waste, (HLW)*—includes spent nuclear fuel and solid wastes obtained on conversion of wastes resulting from the reprocessing of spent nuclear fuel and other wastes as approved by the NRC for disposal in a deep geologic repository.

3.2.7 *waste form*—the radioactive waste materials and any encapsulating or stabilizing matrix in which it is incorporated.

3.2.8 *waste package*—the waste form and any containers, shielding, packing and other absorbent materials immediately surrounding an individual waste container.

3.2.9 *data*—information developed as a result of scientific investigation activities , including information acquired in field or laboratory tests, extracted from reference sources, and the results of reduction, manipulation, or interpretation activities conducted to prepare it for use as input in analyses, models or calculations used in performance assessment, integrated safety analyses, the design process, performance confirmation, and other similar work.

3.2.10 *scientific investigation*—any research, experiment, test, study, or activity that is performed for the purpose of investigating the material aspects of a geologic repository, including the investigations that support design of the facilities, the waste package and performance models.

3.2.11 *technical information*—information available from drawings, specifications, calculations, analyses, reactor operational records, fabrication and construction records, other design basis documents, regulatory or program requirements documents, or consensus codes and standards that describe physical, performance, operational, or nuclear characteristics or requirements.

3.2.12 *risk-informed*—refers to an approach to the licensing of a geologic repository based on the understanding that some risk will always exist and that the engineered barrier system and natural barrier system are designed to perform such that the risk is acceptable.

3.2.13 *risk-significant*—pertaining to an engineered barrier system material that has been determined to have a significant effect on the performance of the repository during the regulatory compliance period after closure.

3.2.14 *boundary dose risk*—the quantitative estimate of the expected annual dose to an individual at the repository site boundary over the compliance period weighted by the probability of occurrence. **(10 CFR 63.113)**

3.3 *Definitions of Terms Specific to This Standard*—The following definitions are defined only for the usage in this standard, and for the explanation of the analyses contained herein.

3.3.1 *accelerated test*—a test that results in an increase in the rate of an alteration mode or in the extent of reaction progress, when compared with expected service conditions.

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[5] Available from U.S. Government Printing Office Superintendent of Documents, 732 N. Capitol St., NW, Mail Stop: SDE, Washington, DC 20401, http://www.access.gpo.gov.

[6] See *Compilation of ASTM Standard Definitions*, available from ASTM Headquarters, 100 Barr Harbor Drive, West Conshohocken, PA 19428.

Changes in the expected alteration mechanism(s) caused by the accelerated test conditions, if any, must be accounted for in the use of the accelerated test data.

3.3.2 *alteration*—any change in the form, state, or properties of a material.

3.3.3 *alteration mechanism*—the fundamental chemical or physical processes by which alteration occurs.

3.3.4 *alteration mode*—a particular form of alteration, for example, dissolution or passivation.

3.3.5 *analog*—a material, process, or system whose composition and environmental history are sufficiently similar to that anticipated for the materials of interest to permit use of insight gained regarding its condition or behavior to be applied to a material, process, or system of interest.

3.3.6 *attribute test*—a test conducted to provide material properties that are required as input to behavior models, but that are not themselves responses to the environment. Examples are density, thermal conductivity, mechanical properties, radionuclide content of waste forms, etc.

3.3.7 *behavior*—the response of a material to the environment in which it is placed.

3.3.8 *bounding model*—a model that yields values for dependent variables or effects that are expected to be either always greater than or always less than those expected for the variables or effects to be bounded.

3.3.9 *characterization test*—in high-level radioactive waste management, any test or analysis conducted principally to furnish information used to determine parameter values for a model or develop a mechanistic understanding of alteration. Examples include polarization tests, solubility measurements, etc.

3.3.10 *confirmation test*—a test in which results are not used in the initial development of a model or the determination of parameter values for a model but are used for comparison with the predictions of that model for model validation.

3.3.11 *degradation*—any change in a material that adversely affects the behavior of that material or its ability to perform its intended function; adverse alteration.

3.3.12 *empirical model*—a model based only on observations or data from experiments, without regard to mechanism or theory. An empirical model may be developed from a direct fit of the experimental data such as a regression analysis or may be developed as a model which encompasses all the observed data points; that is, a bounding model.

3.3.13 *extrapolation*—the act of predicting long-term material behavior beyond the range of data collected by empirical observation in short-term tests.

3.3.14 *in-situ test*—a test conducted in the geologic environment in which a material or waste form will be emplaced.

3.3.15 *model*—a simplified representation of a system or phenomenon, based on a set of hypotheses (assumptions, data, simplifications, and/or idealizations) that describe the system or explain the phenomenon, often expressed mathematically.

3.3.16 *predict*—declare in advance the behavior of a material on the basis of a model.

3.3.17 *mechanistic model*—model derived from accepted fundamental laws governing the behavior of matter and energy. It corresponds to one end of a spectrum of models with varying degrees of empiricism.

3.3.18 *pyrophoric*—capable of igniting spontaneously under temperature, chemical, or physical/mechanical conditions specific to the storage, handling, or transportation environment

3.3.19 *semi-empirical model*—a model based partially on a mechanistic understanding and partially on empirical fits to data from experiments.

3.3.20 *service condition test*—a test with a material that is conducted under conditions in which the values of the independent variables characterizing the service environment are within the range expected in actual service.

3.3.21 *model validation*—the process through which model predictions are compared with independent measurements or analyses to provide confidence that a model accurately predicts the alteration behavior of waste package/EBS materials under particular sets of credible environmental conditions. This provides confidence in the capability of the model to predict alteration behavior under conditions or durations that have not been tested directly. An alteration model that has been demonstrated to provide bounding results under all credible environmental conditions, and is used to provide bounding values for the alteration behavior, may be regarded as validated for its intended usage.

4. Summary of Practice

4.1 This practice covers the general approach for proceeding from the statement of a problem in prediction of long-term behavior of materials, through the development, validation, and confirmation of appropriate models, to formulation of actual predictions.

5. Significance and Use

5.1 This practice supports the development of materials behavior models that can be used to predict alterations in materials over the very long time periods pertinent to the operation of a high-level nuclear waste repository; periods of time much longer than can be tested directly. Under the very extended service periods relevant to geological disposal—much longer periods than those encountered in normal engineering practice—equilibrium or steady state conditions may be achieved and models for reaction kinetics may be replaced by models, if justified, describing equilibrium extents of alteration. This practice is intended for use for waste form materials and materials proposed for use in an EBS that is designed to contain radionuclides released from high-level nuclear waste forms as they degrade over tens of thousands of years and more. Various U.S. Government regulations pertinent to repository disposal in the United States are as follows:

5.1.1 Public Law 97–425, the Nuclear Waste Policy Act of 1982, provides for the deep geologic disposal of high-level radioactive waste through a system of multiple barriers. The radiation release limits are to be set by the U.S. Environmental Protection Agency (EPA) (40 CFR 191). Licensing of such disposal will be done by the U.S. Nuclear Regulatory Commission (NRC).

5.1.2 The analyses described in this Standard Guide can be used to support the demonstration of compliance of the EBS components and design to the applicable requirements of 10

CFR 60 (pertaining to any HLW repository in the U.S.) and 10 CFR 63 (pertaining to the planned HLW repository at Yucca Mountain, NV).

5.1.2.1 10 CFR 60.135 and 60.113 require that the waste form be a material that is solid, non-particulate, non-pyrophoric, and non-chemically reactive, and that the waste package contain no liquid, particulates, chemically reactive or combustible materials and that the materials/components of the EBS be designed to provide – assuming anticipated processes and events - substantially complete containment of the HLW for the NRC-designated regulatory period.

5.1.2.2 10 CFR 63.113 provides that the EBS be designed-such that, working in combination with the natural barriers, the performance assessment of the EBS demonstrates conformance to the annual reasonably expected individual dose protection standard of 10 CFR 63.311 and the reasonably maximally exposed individual standard of 10 CFR 63.312 , and shall not exceed EPA dose limits for protection of groundwater of 10 CFR 63.331 during the NRC-designated regulatory compliance period after permanent closure.

5.1.3 The regulations of the U.S. Environmental Protection Agency (EPA) in Part 191 of Title 40 of the CFR provide that cumulative releases of radionuclides from the disposal system—this refers to the total system performance not just the EBS performance—for the regulatory compliance period after disposal shall have a likelihood of less than one chance in ten of exceeding the values stated for each radionuclide in the regulation. These environmental standards relate to the overall system performance of a geologic repository and they are referred to in NRC requirements of 10 CFR 60.112 and 63.111. Analyses of overall repository system performance may include anticipated and unanticipated events.

5.2 The current governing regulations are 10 CFR 60 as applicable to generic requirements for a repository in the US and 10 CFR 63 as applicable to the proposed repository site at Yucca Mountain. Other site-specific regulations may be required in the development of any alternative or additional US geologic repository site (per 10 CFR 60).

5.3 This practice recognizes that technical information and test data regarding the actual behavior of waste forms and materials that are used in the EBS and exposed to repository conditions for such long periods of time will not be sufficient to develop fully validated models in the classical sense. Rather, the (necessarily) short-term test data acquisition, and use of the data in formulating reliable long-term predictive models, is to be used to support the design, performance assessment, and even the selection of waste package/EBS materials (e.g., low confidence in a degradation model may justify the selection of alternative EBS barrier materials).

5.4 This practice aids in defining acceptable methods for making useful predictions of long–term behavior of materials from such sources as test data, scientific theory, and analogs.

5.5 The EBS environment of interest is that defined by the natural conditions (for example, minerals, moisture, biota, and mechanical stresses) as modified by effects of time, repository construction and operations, and the consequences of radionuclide decay, for example radiation radiation damage, heating., and radiolytic effects. Environmental conditions associated with both anticipated and unanticipated scenarios should be considered.

6. General Procedure

6.1 *Development of Modeling Approach*:

6.1.1 Fig. 1 outlines the logical approach for the development of models for the prediction of the long-term behavior of waste form and EBS materials in a repository. The major elements in the approach are problem definition, testing, modeling, prediction, and confirmation. It is not expected that Fig. 1 will apply exactly to every situation, especially as to the starting point and the number and type of iterations necessary to obtain validated alteration models. However, it is likely that development of models will contain these major elements. Details on these elements are given in Sections 7-26. Development of predictive models will likely be conducted under a quality assurance program as discussed in Section 27. An important aspect of predictive models is determination of the uncertainty of the model , including uncertainties in the form of the model (that is, how well the model represents the physical system or process), uncertainties in the data used to determine model parameters, uncertainties in the predicted environmental service conditions to which the model is applied, etc. The consequences of these uncertainties with regard to the performance of the disposal system are used to determine the risk.

6.2 *Identification of Risk-Significant Waste Form and EBS Material Behavior Characteristics*:

6.2.1 Using a risk-informed approach to repository performance assessment, those waste form and engineered barrier materials behavior characteristics that may substantially contribute to risk (by affecting the release of radionuclides from the repository over the regulatory compliance period) are included in the final performance assessment. However, the repository operator must perform initial performance assessments to analyze the sensitivity of specific materials alteration processes to fully identify those barriers that are important to safety and those barriers that are important to waste isolation. It is the long-term behavior of these risk-significant materials that is the subject of this procedure. Criteria for identifying materials that may be risk-significant are the following:

6.2.1.1 Materials, systems, structures, components, and barriers that are depended on to contain the waste form within the repository environment,

6.2.1.2 Materials, systems, structures, components, and barriers that are deployed to protect the containment of the waste form, and

6.2.1.3 Natural barriers that hold up release of waste radionuclides in the event of containment material failure and waste form degradation.

6.2.2 EBS and waste form materials whose degradation characteristics are determined to be unimportant to waste isolation should be evaluated to determine their useful lifetimes and expected performance, but their behavior models may not need to be as mechanistically based as those important to waste isolation.

6.3 *Identification of Credible Ranges for Environmental Conditions*:

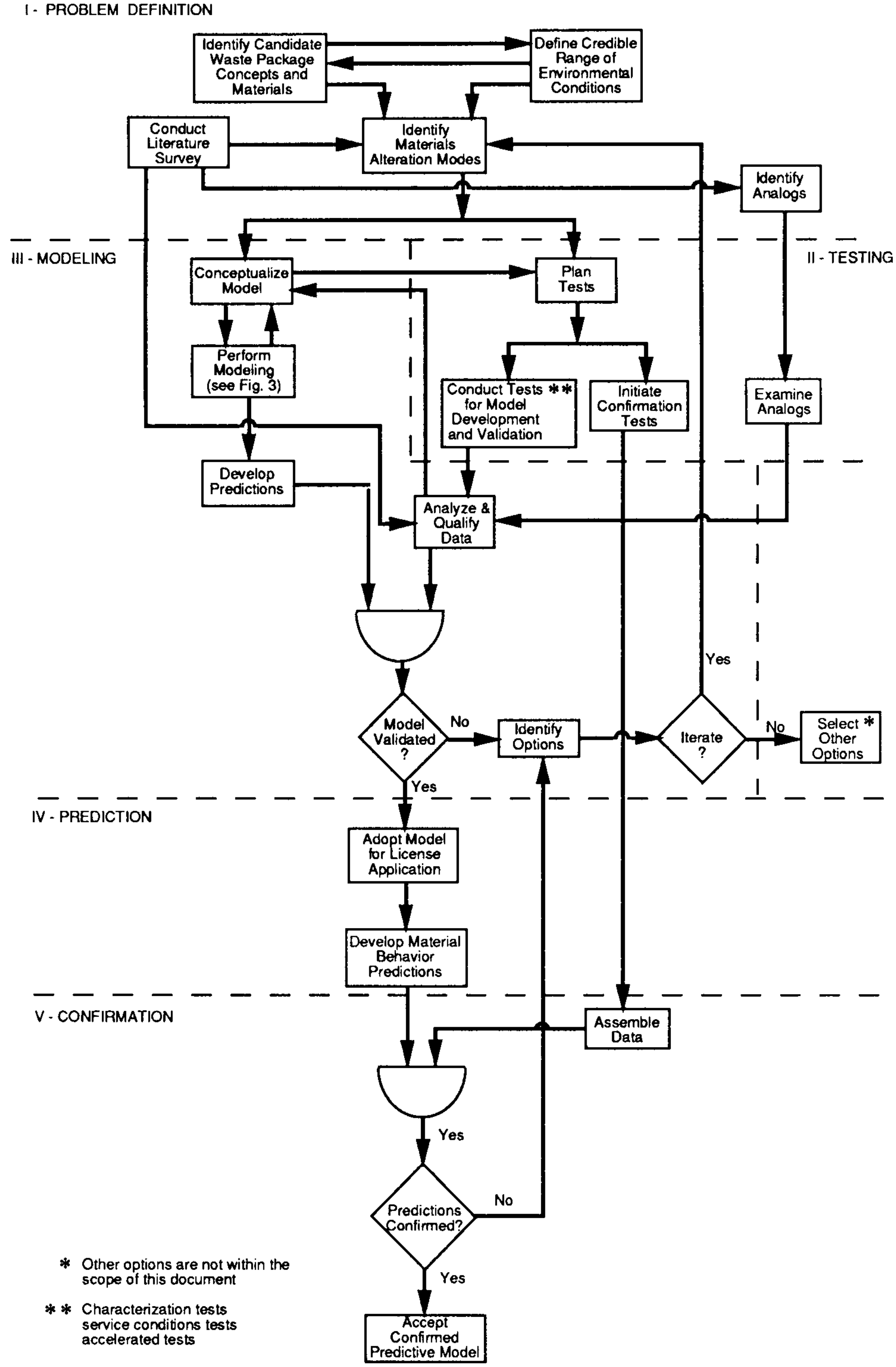


FIG. 1 Logic for the Development of Predictive Models for the Post-Closure Behavior of Waste Package Materials

6.3.1 The behavior of a material will depend on the environment in which it is used. The environment within a disposal system will be affected by both the natural conditions and the effects of EBS components. For example, corrosion of EBS materials and radiolysis will significantly alter the chemistry of the groundwater that contacts the waste forms. The anticipated range of repository environments should be defined and validation of model predictions be done over this range. Tests conducted under conditions outside this range could serve as accelerated tests.

PROBLEM DEFINITION

7. Scope

7.1 Problem definition includes evaluation of the following issues that are important in the development of models to support predictions of long-term behavior of repository materials:

7.1.1 Identification of potential environmental conditions to which the materials may be exposed,

7.1.2 Identification of possible waste-package design concepts,

7.1.3 Identification of waste package materials, including waste forms,

7.1.4 The identity, composition, and condition of the waste forms and important radionuclides,

7.1.5 Identification of potential materials alteration modes,

7.1.6 Identification of appropriate natural analog materials, and

7.1.7 Literature surveys and other sources of information helpful in characterizing the alteration of EBS and waste package materials.

7.2 The objective of the problem definition approach is to identify the processes and interactions that should be included in the predictive model and possible alteration modes. This information is used to design conceptual models and design tests to develop and evaluate process models.

7.3 In this practice, methods are recommended for the development of predictive models for long-term alterations of EBS and waste package materials, including waste forms, that are proposed for use in the geologic disposal of high-level radioactive wastes. This practice recommends a methodology for assessments of performance of materials proposed for use in systems designed to function either for containment or control of release rates of radionuclides.

7.4 This practice outlines a logical approach for predicting the behavior of materials over times that greatly exceed the time over which direct experimental data can be obtained. It emphasizes accelerated tests and/or the use of models that are based on an appropriate mechanistic understanding of the processes involved in long-term alterations of materials used under repository conditions.

8. General Considerations

8.1 *Site Characterization*—A potential repository site must be investigated with respect to its geologic, hydrologic, seismic, etc. conditions. For purposes of this practice, site characterization includes the identification of likely impacts of the environmental conditions on the behaviors of the waste form and EBS materials (see 8.5.1, 9.1, and 10.2).

8.1.1 *Environment*—The geologic environment shall be evaluated by characterization of the initial environment and mechanical condition and consideration of the effects of time and alteration of EBS and waste form materials on the environment. Ranges in the values of such environmental conditions as temperature, groundwater chemistry, and colloid content may be needed to account for changes in the environmental conditions that occur over time.

8.2 *Conceptual Designs*—A general concept for an EBS design is devised to meet regulatory requirements. Specific designs for the components of the EBS are developed based on current understanding of the conditions of a particular site and the waste package design.

8.3 *Materials Identification*—From the initial concepts and investigations of a repository site, candidate EBS and waste package component materials are proposed based on the geologic environment and the conceptual design. Since these materials serve the function of containment and control of potential radionuclide release rates, their alteration behavior under the set of conditions expected in the repository over long time periods must be reliably determined and the alteration modes understood. This understanding is developed by first reviewing both the available information regarding the environmental conditions and the effects of the environment on the candidate materials.

8.3.1 Information regarding natural analogs might be available to provide early guidance for the selection of EBS component materials and/or the long-term alteration of these and waste form materials in the repository environment.

8.3.2 The selection of WP/EBS materials for waste package and/or EBS application, or the way in which waste forms are configured within a waste package, could also be influenced by the level of validation attainable for the degradation rate model. This approach could lessen the need for hard-to-achieve high confidence levels in a degradation model. For example, a container material that exhibits a moderate but predictable rate of general corrosion, but is not susceptible to localized corrosion, might be selected for use as a corrosion barrier and the thickness of the wall engineered to provide for a 'corrosion allowance.'

8.4 *Ranges of Materials Properties and/or Environmental Conditions*—Preliminary descriptions of the materials to be tested shall be used to determine their physical and mechanical properties. Frequently, a range of values will be needed to specify parameters used to characterize materials.

8.4.1 *Ranges*—A range of parameter values for environmental conditions or material properties may be used to account for uncertainty in the anticipated temporal and spatial variability in the environmental condition, etc. The waste forms themselves will likely have to be described by ranges to take into account differences in properties due to variations in composition production history, product usage, process control, etc.

8.4.2 *Bounding Conditions*—Bounding conditions represent the anticipated extreme credible values of a range of parameter or variable values. These furnish necessary input for making predictions of performance limits. However, thorough evaluations of the alteration mechanisms, all important material attributes, and the effects of these attributes on the anticipated alteration processes are required to ensure that the calculations with bounding conditions do provide performance limits. For example, the pH value that gives the lower limit of the glass dissolution rate may not be the extreme of the range of environmental pH values.

8.5 *Preliminary Testing*—A substantial amount of data related to both the materials of interest and the extant environmental conditions may be available before the initiation of tests for model development. Various preliminary modeling and testing efforts can be conducted to understand specific aspects of the material/environment system and make preliminary predictions of the alteration processes. Insight gained from the preliminary tests and predictions can be used to design characterization and accelerated tests for use in the development of the model for long-term predictions.

8.5.1 *Interactions*—The process of predicting materials behavior in repositories must involve consideration of interactions between materials and complex environments. For example, interactions between various materials and the environment may lead to the formation of reaction products that, in turn, become part of the environment. Interactions between different materials within the EBS may be direct, in the case of materials that are in physical contact, or indirect through the groundwater chemistry. That is, changes in the groundwater due to corrosion of one material will affect the corrosion behavior of other materials that the groundwater contacts. Characterization tests should be conducted to ensure that the range of environmental parameters captures these effects. The presence of microbes and effects of seismic events, etc., should also be considered in estimates of environmental conditions.

8.6 *Literature Survey*—Using the proposed materials and estimates of environmental conditions, a literature survey shall be conducted to obtain insight into possible alteration modes and possibly data that can be used in the development of a model. A literature survey must be conducted to identify and evaluate the usefulness of any analogs for later validation activities.

8.7 *Preliminary Models*—For each important alteration process, preliminary models shall be developed to represent and evaluate steps in the process, postulates, and inferences related to either observed or expected behavior of the materials in the proposed containment system. These may serve as conceptual models.

8.7.1 Inputs to these models can be estimates of values for the independent variables pertinent to environmental conditions and alteration processes or values that are obtained from experiments or other sources. The models are used to estimate pertinent dependent variables, as for example, dissolution rate as a function of time.

9. Specific Procedure—Problem Definition (See Fig. 1)

9.1 *Define Credible Range of Environmental Conditions*—Determine the range of environmental conditions to which the material will be exposed after emplacement. The range should include initial environmental conditions and changes that will occur over time due to changes in climate, radiolysis of air and groundwater, corrosion of EBS components, etc. The extent of such interactions may be difficult to quantify initially, but should be noted and accounted for in a final model.

9.2 *EBS Conceptual Design*—Establish the design concepts of the EBS and propose the functional and spatial relationship for the various components.

9.2.1 If viable options exist in the EBS conceptual design, the effects of each can be incorporated into subsequent modeling and testing steps. For example, consider the values of parameters that will differ depending upon whether emplacement geometry is vertical or horizontal.

9.3 *EBS Materials*—Identify the types and intended uses of all the materials that comprise the EBS components. This would include, for example, identification of weldments and the processes and materials with which they are to be fabricated.

9.4 *Literature Survey*—Use technical literature to help identify alteration modes for the materials of interest relevant to the environmental conditions for the repository site being evaluated.

9.5 *Variables*—Identify the variables regarded to be important to material behavior, for example, the amount of water expected to contact a waste glass. For each independent variable, attempt to identify the expected range of values. Confirm that excluded variables have negligible effect.

9.6 *Mechanisms for Alteration Processes*—For each alteration process, identify possible alteration mechanisms. For example, glass may be altered by dissolution and precipitation processes that convert the glass to phases that are thermodynamically stable. For the alteration mode of glass dissolution, one can describe an alteration mechanism that includes water diffusion into the glass and various reactions associated with ion-exchange and hydrolysis. For precipitation processes, an alteration mechanism for the formation of alteration phases could include precipitation from solution or transformation of a gel.

9.7 *Analogs*—Identify potential analogs for materials, processes, or systems. These may be either natural or man-made.

9.7.1 Identify the aspect of the analog that can be compared with the material or process under consideration. Differences will likely exist between the compositions of the analog and the repository material and the environment to which they are exposed. Evaluations of the significance of the differences may be used to support or disqualify use of the analog as a means for validation of the alteration model.

TESTING

10. Scope

10.1 Testing of waste form and EBS materials is required to establish whether these materials will effectively contain radionuclides for the containment period. Tests are conducted to develop models that can be used to predict materials behavior over time periods longer than can be tested directly. Tests conducted over a comparatively short period, for example, less than 20 years, will be used to support development of predictive behavior models for the response of the materials to the repository environment for the regulatory compliance period. The testing program must address the development, validation, and confirmation of these models.

10.1.1 Materials testing programs should be designed with the goal of supporting the development and application of materials behavior models, as well as the minimizing the uncertainties in the test data, the models, and the use of the models in calculations of long-term behavior in an EBS.

10.2 The testing concepts described herein do not specifically address the testing of integrated systems of the EBS; those systems are expected to be tested in later stages of repository development. This practice does not address testing required to define (or model) the repository environment (that is, the groundwater quantity or chemistry, host rock properties, etc.).

10.3 *Purpose of Testing*—Testing of EBS materials will be required for a variety of reasons, some of which are listed below.

10.3.1 Establish a database for the properties of waste form and EBS materials, especially the properties required in evaluations in reliability and uncertainty in behavior models.

10.3.2 Evaluate the possible modes and mechanisms of alteration.

10.3.3 Simulate, in a short period of time, the state of a material in the repository environment after long periods of time, for example, produce an artificially "aged" material.

10.3.4 Examine analogs to identify alteration modes and to obtain data on alteration rates.

10.3.5 Provide data on the interactions between components of an EBS.

10.3.6 Select values for independent variables–these are the parameters used in models.

10.3.7 Provide evaluations of reliability and uncertainty as needed to validate the models.

10.3.8 Provide confirmation test data to furnish further proof of the validity of predictions made using models of materials behavior. Confirmatory data is required to be taken during the repository pre-closure period.

11. General Testing Considerations

11.1 *Types of Tests*—The tests listed in 1.1.3 are described in more detail in Sections 12-17. A single test method can simultaneously serve more than one function. For instance, a single test procedure could serve as both a characterization test and as an accelerated test depending on the test parameters that are used. The tests may be applied to analog materials to provide insight into long-term mechanisms of alteration.

11.1.1 *Attribute Tests*—These are sometimes needed to provide input to models of materials alteration. Included are any tests or measurements of intrinsic materials properties that do not depend on the environment the material is exposed to, such as density, specific surface area, thermal properties, grain size, hardness, tensile strength, etc. These properties could be used indirectly to support the alteration model. For example, the Product Consistency Test-Method A (Test Methods C 1285, PCT-A) can be considered an attribute test when used for the purpose of demonstrating HLW glass product consistency, and therefore the applicability of the alteration model to it.

11.1.2 *Tests for Model Development and Validation*—Characterization tests, accelerated tests, and service condition tests have the common purpose of providing data to support the development of material alteration models and behavior predictions for the repository post-closure period. Close coordination between testing and model development can facilitate the validation of models.

11.1.2.1 Service condition tests are used to determine what material alteration processes are likely to be important during the service life of the disposal system.

11.1.2.2 Characterization tests are designed to establish alteration mechanisms for important processes, measure the effects of environmental variables on material alteration, and develop model parameter values. For example, the PCT-A (Test Methods C 1285) could be considered a characterization test when used to provide data for the development or regression of model parameters.

11.1.2.3 Accelerated tests are designed to increase the reaction progress by either increasing the rates of reactions and processes or increasing the rate of alteration in the environmental conditions relative to anticipated service conditions, without changing the mechanism of the alteration. For example, tests can be conducted at temperatures higher than expected in the disposal system to increase the dissolution rate of a material.

11.1.3 *Confirmation Tests*—Confirmation tests are expected to be conducted over extended times and they are intended primarily to validate materials alteration models that have already been developed. Confirmation tests are performed after the initial development of models following the procedures of this practice.

11.2 *Behavior Model*—The alteration of waste form and EBS material can be predicted using a behavior model developed from characterization tests, accelerated tests, service condition tests, literature analyses, and analyses of analogs. Values of fitting parameters of the model may be obtained by using regression analyses on the data obtained from accelerated, characterization, and/or service-condition tests.

11.2.1 The analytical form (Arrhenius, constant rate, polynomial, etc.) of the behavior model will determine the confirmation tests used to validate it. For example, an alteration mode having an Arrhenius form may require that tests be conducted over a range of temperatures; preferably the range of temperature bounds the anticipated service condition temperatures.

11.2.2 The ability of the behavior model to provide reliable predictions will be strongly dependent on the uncertainties in the mathematical form of the model itself (for example, the degree to which the model is based on a mechanistic understanding of the alteration process), uncertainties in the test data used to derive the fitting parameters of the model, and the uncertainties in the actual in-service conditions for which the model is applied (see Section 24 on Uncertainties). Knowledge concerning these uncertainties would aid in the evaluation of test data to be used in model development.

11.2.3 The reliability of model predictions will depend upon both how well the model represents the alteration mechanism under the in-service conditions (for example, type or stoichiometry of corrosion product, form of alteration layers, mode of degradation) and how well the values of environmental variables used in the model represent the in-service environmental conditions (for example, temperature, groundwater chemistry, groundwater quantity).

12. Attribute Tests

12.1 *General*—The prediction of the response of materials to the repository environment during the post-closure period will require the specification of materials properties ("attributes") that are not themselves responses to the repository environment. These properties are not time dependent and may be used as input to the behavior models.

12.1.1 Examples of such properties are density, thermal conductivity, chemical composition, radionuclide content, mechanical properties, etc.

12.1.2 Attribute tests are designed to provide specific information on test materials when necessary for the development of the behavior models and when reliable data are not available from the literature. It is expected that most of the required information concerning spent fuel and high level waste material attributes will be available in the literature.

12.2 *Specific Procedure-Attribute Tests*:

12.2.1 Formulate a behavior model for an alteration mode of interest (see Modeling section).

12.2.2 Identify the material properties required to apply the model.

12.2.3 Examine the literature for materials properties and evaluate which properties may be unambiguously determined without testing.

12.2.4 Perform attribute tests on those properties for which unambiguous values could not be determined from the literature.

12.2.5 Compile the values for all properties necessary as input to modeling.

13. Characterization Tests

13.1 *General*—Characterization tests have the primary function of providing a mechanistic understanding of the important processes of material alteration expected in the repository environment and measuring model parameter values. These tests are used to establish both the suitability and the basic form of the behavior model.

13.1.1 *Purpose*—Characterization tests are designed to identify waste form and EBS alteration mechanisms that could occur in a repository.

13.1.2 Test conditions may depart significantly from the expected repository conditions, and so it may be necessary to investigate the sensitivity of the alteration mechanisms to variations in the values of particular test parameters.

13.1.2.1 Examples of these tests include anodic polarization tests, radionuclide solubility measurements, x–ray diffraction analyses, etc.

13.2 *Specific Procedure-Characterization Tests*:

13.2.1 Identify the candidate EBS material and the credible range of in-service environmental parameters such as temperature, groundwater chemistry, and groundwater flow.

13.2.2 Use literature analyses, analogs, scientific judgment, and experience to postulate potential material alteration modes and mechanisms.

13.2.3 Perform tests to identify alteration mechanisms that could plausibly occur in the repository environment.

13.2.4 Analyze the information from the characterization tests, both quantitative and qualitative, and identify the alteration mechanism(s) expected in the repository environment.

13.2.5 Identify parameters that could be used to accelerate the rate of alteration without changing the alteration mechanism.

13.2.6 Integrate the results of characterization tests with the behavior modeling (see Modeling section).

14. Accelerated Tests

14.1 *General*—The purpose of this type of test is to increase the rate of one or more alteration modes or the reaction progress without changing the basic alteration mechanism(s) of the alteration mode under investigation. Therefore, some knowledge of the mechanism that is operative under in-service conditions is needed for the design of the accelerated test and meaningful use of accelerated test data. Processes may be accelerated by increasing various test parameters, including temperature, material surface area, particle size, or roughness, solution volume and flow rate, solute concentrations, humidity, etc., relative to their in-service values.

14.1.1 If the alteration mechanism that is operative in the accelerated test differs from that which is operative under the in-service conditions or changes over a range of accelerating test conditions, the accelerating test conditions must be reevaluated.

14.1.1.1 For example, if higher-than-repository temperatures are used to accelerate the rate of corrosion of a material, and during the tests the corrosion product is found to change from *A* (which forms at repository-relevant conditions) to *B* (which forms at the higher temperatures), the investigator may not be able to use the *B* rate data in the rate model for *A*. If *B* is judged to be due to a possible alternative reaction in the repository environment, a new corrosion model must be formulated incorporating its formation, and the *B* data may possibly be used to calibrate this new model. Otherwise, the *B* data are not relevant to the behavior model.

14.1.2 *Use*—Accelerated tests may be used to:

(1) Alter the state of a material in a short time to simulate long time repository exposures, and thereby produce artificially "aged" materials. (This may be desirable for determining the attributes and characteristics of materials after long exposures to potential repository conditions, or for testing the response of "aged" materials to possible changes in the repository conditions during the post-closure period),

(2) Measure the rates of slow reactions,

(3) Promote the formation of alteration phases for identification and characterization,

(4) Promote the approach to solution saturation, and

(5) Age the solution that contacts the material to represent conditions that may occur after long reaction progress.

14.1.2.1 An example is the exposure of samples of spent fuel to conditions that accelerate alteration relative to service conditions (such as high temperature, crushing to expose grain boundaries, etc.) to obtain upper limit values for radionuclide release upon exposure to groundwater in the post-contaminated period. The effects of the accelerating conditions should be quantified and mechanistically described.

14.1.3 *Synergistic or Competing Effects*—Because of the potentially large number of independent variables (for example, temperature, radiation, mechanical stress, groundwater chemistry, and material condition), careful consideration should be given to possible synergistic and/or competing effects.

14.1.4 *Models*—Results of accelerated tests can be used to develop or support a behavior model by verifying a null result at extreme conditions, or by verifying a parameter in the alteration model.

14.1.4.1 As an example of verifying a null result, a test for stress corrosion cracking (SCC) of a candidate waste container material might be conducted to establish that SCC initiation can occur only under temperature and water chemistry conditions well beyond that which can plausibly occur in the repository. The test could also establish that even under high temperatures and aggressive water chemistry a stress corrosion crack would not initiate.

14.1.4.2 An example of verifying a parameter in a proposed alteration model might be a test for general corrosion that is conducted under higher temperatures than expected in the repository or higher levels of anodic polarization. From the data, best-fit values could be obtained for making a determination of an activation energy for diffusion across the corrosion layer and the free energy of formation of the corrosion product based on a mathematical model for general corrosion that incorporates diffusion and reaction processes. In each of the above examples, the accelerated test results can "validate" the use of the model.

14.1.5 Fig. 2 shows the steps involved in the development and performance of accelerated tests. The figure also demonstrates the necessary connection between testing and modelling, in the development of a reliable behavior model. In general, the steps given in 14.2 should be followed.

14.2 *A Specific Procedure for Accelerated Testing*:

14.2.1 Define the alteration mode to be accelerated.

14.2.2 Identify key alteration indicators (for example, extent of corrosion, pitting, weight loss).

14.2.3 Identify the type of test(s) and range of test conditions (the parameters needed in models) to be used in the accelerated test.

14.2.4 Identify possible alteration mechanisms and formulate preliminary alteration model.

14.2.5 Postulate how the alteration mode can be accelerated.

14.2.6 Perform tests using a prescribed set of parameters, that is over a selected range of test conditions.

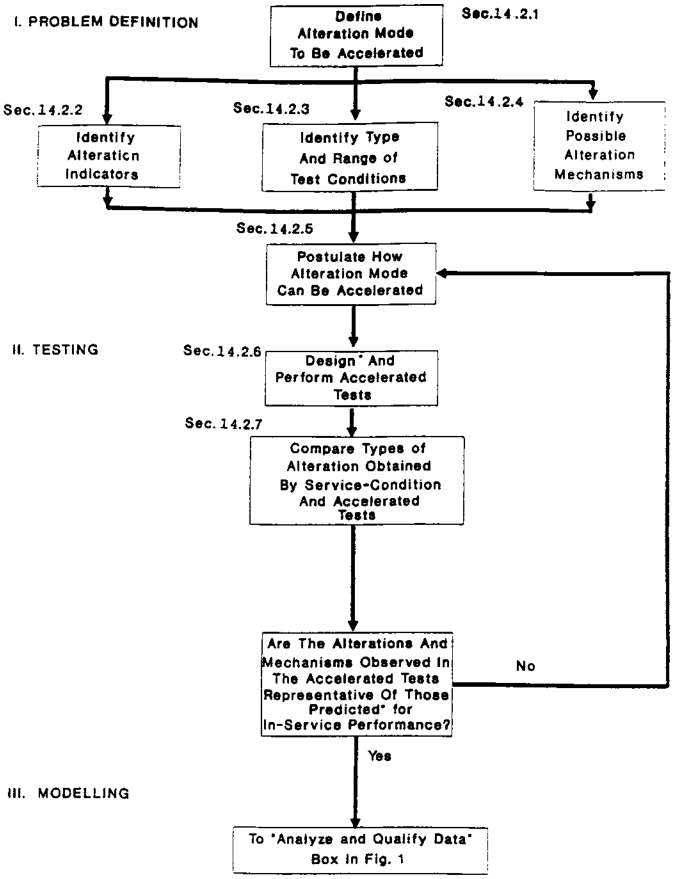
14.2.6.1 Compare the types (mode and extent) of alteration attained in accelerated tests with those attained in service-condition tests and those represented in the behavior model.

14.2.6.2 Verify that the alteration mechanisms of accelerated tests are like (or applicable to) the expected mechanisms under repository conditions.

14.2.7 Identify alteration mechanisms and the range of test conditions (the parametric values) under which these mechanisms apply, and compare mechanisms with those postulated in 14.2.4.

14.2.7.1 Show that these mechanisms are expected to persist over a pertinent range of values for parameters, including the service term, taking into account anticipated changes in the environment to which the materials of interest are exposed.

14.2.7.2 If the alteration mechanisms (or modes) of the accelerated tests differ from those of the model, reevaluate the model and the accelerated test conditions for relevancy to repository conditions and return to 14.2.5 to iterate on this process until a satisfactory accelerated test is developed.



* Based on the results of characterization tests, service condition tests, and literature data.

FIG. 2 Recommended Procedure for Developing Accelerated Tests for Waste Package Component Materials

14.2.8 Provide results as input to the modelling activity.

14.2.9 Determine whether the extent of alteration is acceptable for the particular material in actual service.

15. Service Condition Tests

15.1 *General*—The purpose of service condition testing is to establish a suitable database for determining the alteration mechanism of EBS materials under repository-relevant conditions, and for determining (for example, regressing) model fitting parameters.

15.1.1 These tests are used to identify the key aspects of the materials and the environment that affect the alteration mechanisms under expected conditions. Observations of the alteration mechanisms under service conditions can then be used to determine the relevance of accelerated tests (and the mechanisms observed therein) to alteration model development.

15.1.2 Service condition tests should be designed to show the dependence of material behavior on relevant environmental conditions and identify important environmental variables. Service condition tests should be conducted over the full expected range of repository environmental conditions.

15.1.3 Service condition tests establish reference test and material behavior conditions as a basis for long-term confirmation testing (see Section 13).

15.1.4 Service condition tests may provide data on alteration of materials under actual repository test conditions by use of short-term *in-situ* tests (for example, tests conducted in the repository exploratory studies facility) for model validation.

15.1.5 The configurations of service condition tests are likely to be similar to those of the confirmation tests (as described in Section 17) with the primary difference being the test duration. The duration of a service condition test that serves the purpose of model development and validation may be extended to serve model confirmation purposes (see Note 2 and Fig. 1).

15.2 *Specific Procedures-Service Condition Tests*:

15.2.1 Select test conditions. "Normal" conditions may be defined in terms of a range that includes the expected average values for each material and environmental variable along with maximum and minimum values of these variables. Results obtained under "normal" conditions may be used as reference values.

15.2.1.1 Plan tests to establish a sufficiently comprehensive database.

15.2.1.2 Conduct sufficient number of tests to measure the responses for the full range of "normal" conditions. Note that the most severe conditions may not yield the maximum response.

15.2.1.3 Compile and evaluate the data obtained and develop models using the best mechanistic understanding of alteration behaviors.

16. Analysis and Testing of Analogs

16.1 *General*—When long-term predictions are made based on mechanistic models obtained using the results of characterization, accelerated, and service condition tests, confidence in the validity (of the predictions) over many thousands of years could be considerably enhanced through the analyses of analogs, both natural and man-made.

16.1.1 *Choice*—Analogs should be chosen with the understanding that it is likely that no perfectly matching analog will be found. For example, no compositional analog to stainless steel is expected, but iron objects, including some quite rich in nickel, exist and may have some applicability to selected alteration behaviors.

16.1.2 The analyses of analogs can be crucial in determining whether different mechanisms can control alteration modes over long time periods.

16.1.3 *Use*—Natural and man-made analog materials can serve as the test specimens for the characterization tests described in Section 13 and the accelerated tests described in Section 14. The analogs provide confidence in an experimental method for accelerating corrosion behavior and in the model used for particular alteration modes.

16.1.3.1 The proper use of analogs requires having reliable information concerning their age, chemical composition, etc. (that can be determined by means of the attribute testing described in Section 10) and their conditions of exposure, such as leachant compositions, contact time, etc. Determinations of these types of information are outside the scope of this practice.

16.1.3.2 It is unlikely that analogs will be found that are identical in composition and conditions of exposure to the waste-package materials in the repository. For example, natural uranium minerals might be used as analogs for the alteration of uranium dioxide spent fuel, but such an analysis should recognize that such minerals did not evolve in a geochemical environment that included close proximity to zirconium metal. A good use of analogs would be to help validate model predictions over a range of material and groundwater conditions.

16.1.4 Characterization of the short-term behavior of analog materials in laboratory experiments could be used to establish that the analogs behave similarly in natural and experimental environments. This would support the conclusion that all relevant mechanisms have been taken into account in the model.

16.2 *Specific Procedure-Analysis and Testing of Analogs*:

16.2.1 *Literature Search*—Search existing literature for potential analogs. Include work in other areas such as archaeometallurgy, geology, and history.

16.2.1.1 Identify, if possible, potential natural or man-made analogs appropriate for the material and alteration mode under investigation.

16.2.1.2 Analyze the degree of similarity and justify the usefulness of the analog in providing information for the alteration mode of interest.

16.2.2 *Samples*—Obtain multiple samples of the proposed analog materials, including samples of differing ages and differing degrees of alteration, if available.

16.2.3 Characterize the site where the analogs were found, for example:

16.2.3.1 Dating of site,

16.2.3.2 Geology of site and depth of burial,

16.2.3.3 Sample storage conditions following retrieval, and

16.2.3.4 Site environment (soil, precipitation, air, etc.).

16.2.4 Characterize the analogs, including:

16.2.4.1 Photographic documentation of specimens and of retrieval process,

16.2.4.2 Dating of specimens and time of exposure,

16.2.4.3 History of specimens and environmental exposure, including nature of leachant, contact time, surface volume ratio, temperature, etc.,

16.2.4.4 History of conditions of formation or manufacture, if applicable and available,

16.2.4.5 Chemical composition analysis,

16.2.4.6 Surface analyses (SEM, EDS, etc.), and

16.2.4.7 Structural analyses (microstructure, grain size, crystallinity, size, shape, color, etc.).

16.2.5 Perform attribute, characterization, accelerated, and service-condition tests, as required.

16.2.6 Analyze the data, for example:

16.2.6.1 Estimate the rate of alteration of the analogs,

16.2.6.2 Determine the mechanism(s) of alteration,

16.2.6.3 Compare the data from tests of analogs with data from tests of the candidate materials or waste forms, and

16.2.6.4 Use the results of these data analyses in the development and validation of the models.

17. Confirmation Tests

17.1 *General*—Confirmation tests are designed to produce materials alteration data in order to further support and validate the alteration model after the initial formulation and use of the model for repository license application purposes but prior to final closure of the repository. During the pre-closure period of the repository, testing (particularly *in-situ* testing) should be continued so as to validate key aspects of materials behavior for the waste form and EBS. Also, tests that had begun as service condition tests could be extended, so as to serve the purpose of confirming, over the pre-closure period, the predicted materials alteration behavior.

17.1.1 *Use*—Confirmation tests are used to confirm the model predictions of material behavior over the pre-closure period.

17.1.1.1 They would generally be conducted *in-situ* (such as, within the exploratory shaft facility of the repository) or under conditions expected to be present within the repository. Alternatively, confirmation testing could be conducted to furnish more alteration behavior data than was available during the period of license application analyses. For example, selected parameters could be analyzed for which no data or insufficient data had been made available during initial model validation.

17.2 *Specific Procedure-Confirmation Tests*:

17.2.1 Identify and directly measure repository in-service environmental parameters, such as temperature and groundwater chemistry.

17.2.2 Identify the material alteration mode to be investigated, the manner of testing, and the behavior model to be confirmed.

17.2.3 Perform tests (*in-situ*, as appropriate) and observe the alteration under repository conditions.

17.2.4 Examine material alteration and compare with the predictions of the validated behavioral model (see Confirmation section).

NOTE 1—If the comparison is not satisfactory, it will be necessary to return to the Modeling section of this practice, as this is an iterative process.

17.2.5 Compile confirmation test results and integrate into uncertainty and reliability analyses of long-term behavior model(s).

MODELING

18. Scope

18.1 Modeling may be performed on a risk-informed, performance-based basis to predict the effects of alteration processes on systems, structures, and components that contribute to waste isolation. Modeling may also be performed in support of the production and qualification for repository disposal of high-level waste glass or other manufactured high-level radioactive waste forms.

18.2 A model is used to express the material alteration behavior measured by the responses (the dependent variables) in various tests to variables that have been found to be significant (the independent variables) using mathematical expressions. The objective of modeling in this practice is to predict the long-term behavior of materials based on physical laws, conceptual models, and relatively short-term experimental observations to provide data to fit the model, and insights from natural analogs and physical laws.

18.3 General considerations in modeling are addressed in this practice as well as specific procedures.

19. General

19.1 *Function of Modeling*—Modeling serves at least two functions: demonstration of the self-consistency of data (interpolation) and prediction of long-term behavior (extrapolation).

19.2 *Types of Data Used in Modeling*—This practice provides for the use of several types of information and data in the development and application of models:

19.2.1 Characterization test data,

19.2.2 Accelerated test data,

19.2.3 Service condition test data,

19.2.4 Analog data,

19.2.5 Confirmation test data, and

19.2.6 Established scientific theories and other literature information.

19.3 *Types of Models*—Quantitative models may range from purely empirical to purely mechanistic, depending on the degree to which the mechanisms of the material alteration processes are known.

19.3.1 *Mechanistic Models*—In purely mechanistic models, the relationships between a dependent variable and all independent variables are expressed using mathematical representations for chemical or physical processes. A purely mechanistic model is illustrated mathematically by Eq 1:

$$Y = F(x_1 \dots x_n), \tag{1}$$

where Y is a dependent variable and x_i through x_n are all independent variables that affect Y. The expression $F(x_i)$ represents the exact dependence of Y on the independent variables, and may be comprised of separate terms for the different variables. The dependence of the response on an individual variable x_i is usually determined by evaluating the results of characterization, service condition, and accelerated tests designed to isolate or highlight the effect of that variable.

19.3.1.1 Mechanistic relationships may be identified through first principles and/or a series of tests (usually accelerated, characterization, and service condition tests) to measure the effects of particular variables on specific alteration processes. Mechanisms can be proposed and evaluated for each specific step or process that occurs in the interaction and then combined into an overall mechanism. The proposed mechanism should identify the roles of all variables that significantly affect the alteration rate to be considered as a purely mechanistic model. In most cases, the values of model parameters are extracted from characterization tests conducted specifically for that purpose and verified using other tests in which several variables may affect the material response. For example, if the dissolution rate of a material is known to depend on the temperature, pH, and chloride ion concentration in solution, tests to determine the effect of temperature would be conducted at various temperatures in solutions with constant pH values and chloride ion contents. Likewise, tests to determine the effects of pH and chloride ion content would be conducted at various pH values or chloride ion contents, and at constant temperature and chloride ion content or constant temperature and pH, respectively. Confirmation of the model could be achieved by comparing the measured and predicted responses under particular conditions of temperature, pH, and chloride content that were not used to determine the functional relationships. Distinctions should be made between uncertainties that arise regarding the form of the model, the precision and bias in the test data, and the fitting constants that are extracted from the test data to be used in the model to properly evaluate the total uncertainty in the model predictions (see Section 24).

19.3.2 *Semi-Empirical Model*—Several factors may preclude development of a purely mechanistic model: *(1)* The time and resources required to develop such a model may be impractical. *(2)* An analytical representation of the alteration behavior may not be possible. *(3)* The relationships may be so complex that numerical solutions using the model might not be feasible, even with the fastest computers available. Thus, a purely mechanistic model may be unwarranted, impractical, or unattainable.

19.3.2.1 A semi-empirical model incorporates a mechanistic understanding into the modeling of some processes, while other processes are modeled empirically. Semi-empirical models represent a practical compromise between mechanistic and empirical models. These models are illustrated mathematically by Eq 2:

$$Y = f(x_i \dots x_n) + \epsilon, \tag{2}$$

where Y is the dependent variable and x_i through x_n are the independent variables that have been identified to affect Y. The term $f(x_i \dots x_n)$ represents a plausible but inexact functional expression (or set of expressions) for the relationship between the independent variables and the response. The functional expressions are usually determined by evaluating the results of attribute, characterization, and accelerated tests that isolate or highlight the effect of a particular variable. The residual value e is included in the expression because the function $f(x_i \dots x_n)$ may not fully represent the dependence of the response on the set of variables. This may because it is not possible to determine a functional relationship (either mechanistic or empirical) between some variables and the response, because not all variables are known, because the effects of some variables may not be distinguishable, etc.

19.3.2.2 The approach for developing a semi-empirical model is to postulate a series of steps or reactions as being representative of the processes expected to have the greatest impact on long-term behavior, even though these may not represent the behavior precisely. A relation of the form of Eq 2 can be inferred by scientific reasoning that describes those steps and minimizes the residuals. This is done by conducting characterization tests to measure the effects of important variables and determine the forms of the functions $f(x_i)$. The residual can be expressed as a single value without regard to individual variables or residual values may be identified for each variable.

19.3.3 *Empirical Models*—Purely empirical models describe the observed material responses and dependencies on variables without reference to a mechanism (ME). Purely empirical models appear frequently in the technical literature to quantify identified trends in material behavior. These models often serve as a first step towards the development of a mechanistic model. A possible conceptual empirical model could have the following mathematical form:

$$Y = a_0 + a_1x_1 + a_2x_2 + a_{12}x_1x_2 + \epsilon \tag{3}$$

where Y is the dependent variable, x_1 and x_2 are independent variables, a_0, a_1, a_2, and a_{12} are model coefficients, and ϵ is the residual value. The residual accounts for the possible inexactness of the mathematical expression and included variables for the response. The values of the coefficients and residual are determined using characterization tests with values of the variables that cover their ranges in the service condition. The mathematical form of an empirical relationship between alteration and variables may provide insight into potential mechanisms controlling the alteration. For example, the observation of a dependence on the square root of test duration may be indicative of control by a diffusion process.

19.3.3.1 The approach for empirical models is to obtain a relationship that is consistent with observed data within an acceptable margin of experimental uncertainty. The approach is considered to be purely empirical when no "mechanisms" are postulated or can be inferred from the measured relationship. Variables believed to have an effect on the dependent variable Y are identified and their effects on Y are measured with characterization tests. The correlation between the variable and the response is analyzed to determine a possible functional relationship. The independent variables that affect a particular response may initially be chosen on the basis of judgment, inconclusive data, or some partially applicable theories. Other variables may become apparent during testing. For example, it might be hypothesized that the corrosion rate of a certain steel should be affected by temperature and the concentrations of hydroxyl [OH^-] and chloride [Cl^-] ions in the water to which it is exposed. A possible conceptual model could have the following mathematical form:

$$dY/dt = a_0 + a_1\mathrm{T} + a_2[\mathrm{OH}^-] + a_3[\mathrm{Cl}^-] + a_{23}[\mathrm{OH}^-][\mathrm{Cl}^-] + \epsilon \tag{4}$$

where Y is the extent of dissolution, dY/dt is the dissolution rate, a_0, a_1, a_2, a_3, and a_{23} are model coefficients, and ϵ is the residual values. The expression contains a term to account for a postulated combined effect of the species x_2 and x_3. The coefficients a_0, a_1, a_2, a_3, and a_{23} and the residual ϵ may be obtained by regression of the results of characterization tests conducted under various hydroxyl and chloride ion concentrations that span the range of expected service conditions.

19.3.3.2 The functional forms determined in empirical models may only be applicable under the test conditions used to generate the data. That is, the values of unidentified variables that are taken into account in the residual may be different under different test conditions. In the example in 19.3.3.1, the rate may depend on the carbon content of the steel. The composition of the steel may be taken into account in the value of a_0 or ϵ in the rate expression.

19.3.4 Consider the situation where the dissolution of steel described in the example in step 19.3.3 was dominated by the cross term $a_{12}[OH^-]\cdot[Cl^-]$ and the residual. If the Guldberg and Waage Law of Mass Action is invoked in a second-order kinetic equation, then the Eq 5 may be written:

$$dY/dt = k[OH^-]^{\alpha}\,[Cl^-]^{\beta} \qquad (5)$$

19.3.4.1 This relates the reaction rate to the product of the concentrations of hydroxyl and chloride ions using three parameters. The test data evaluated based on the initial empirical expression can be reevaluated based on the kinetic expression in Eq 5. Additional characterization tests may be required to determine the parameter values.

20. Development of a Materials Behavior Model

20.1 Model development is iterative in nature. As indicated in Fig. 1, the initial step is to formulate conceptual models for the materials alteration modes that were determined to be most important in the problem definition stage based on literature surveys, insight from the behavior of analog materials, etc. The initial conceptual model may be a simplification of the materials alteration behavior or may address a particular process of the overall mechanism. For example, it may be postulated that components are released from a material into solution by a two-stage process of oxidation and dissolution steps. Separate models may be developed and assessed for each stage. The possible impact of neglecting some alteration modes as the conceptual model is developed must be assessed and considered as potential uncertainty in the model. The conceptual model is used to identify information needs and to plan tests to acquire the test data required to use or evaluate the model. These will include attribute, characterization, service condition, and accelerated tests. Fig. 3 shows the modeling process in more detail. Depending on the level of mechanistic understanding of the alteration processes, a model may be considered empirical, semi-empirical, or mechanistic.

20.1.1 Empirical analysis of the conceptual model is usually the initial step because the identities of the significant variables are generally unknown or uncertain. In this case, the data from service condition and characterization tests, and possibly from other sources (for example, attribute tests and natural analogs) are analyzed to identify relationships and trends in the data. The results of calculations with the conceptual model are then compared with the acquired data to evaluate the adequacy of the model and the model is modified as necessary. Another objective of empirical analysis is to look for evidence of changes in the relationship between the independent variables and the response (which may indicate a change in the alteration mechanism) as test variables (for example, temperature and pH) are changed. This aspect is particularly important for the analysis of accelerated test results. Identification of trends in the data during empirical analyses may result in hypotheses of mechanistic relationships. The conceptual model may be modified to take this relationship into account and other experiments conducted to test the hypotheses. The conceptual model may thereby evolve via review by recognized experts in the field into a semi-empirical model using analyses methods such as Expert Elicitation (Note: J.L. Kotra, M.P. Lee and N.A. Eisenberg, USNRC Branch Technical Position on the Use of Expert Elicitation the High-level Radioactive Waste Program, Washington DC 1996.

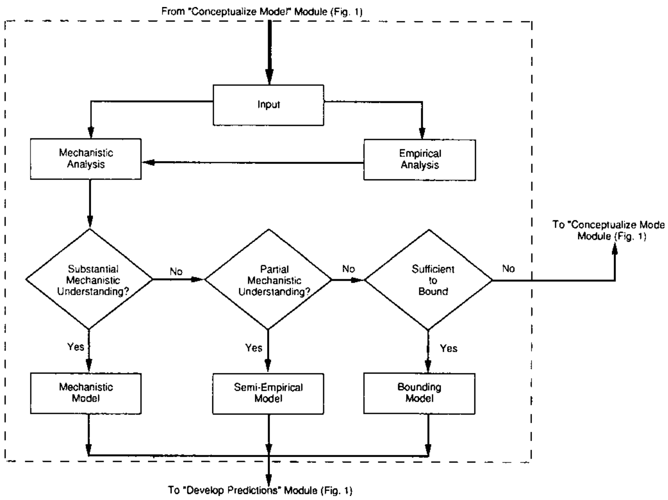


FIG. 3 Details of "Perform Modeling" Module in Fig. 1

20.2 All data used to develop the final process models and determine model parameter values important to waste isolation should be collected in a Quality Assurance (QA)-approved manner (that is, should be qualified). Preliminary tests and analyses used to develop conceptual models do not need to be qualified.

20.3 Data may be rejected on the basis of inadequate test controls or on an objective basis, such as statistical analysis to identify outliers. Data that are not fully qualified may be used if they are the only data available that address a particular issue, are adequate for their intended use in formulating the model, and/or conclusions drawn from them are assigned an appropriate degree of uncertainty.

21. Model Validation

21.1 Model validation is the process through which model predictions are compared with independent measurements or analyses. Validation provides confidence that a model adequately predicts the alteration behavior of waste package/EBS materials under particular sets of credible environmental conditions. Validation provides confidence in the application of the model to predict alteration behavior for conditions that cannot be tested directly. In validating materials alteration models developed using the techniques described above, it should be recognized that "validation" (or proof in the traditional sense) is not fully achievable for the long-term predictions of alteration models. Instead, a reasonable expectation that is based on comparison of the model predictions with service condition, *in-situ*, and confirmation test results and analysis of analogs—and that makes allowance for the long time periods and modeling uncertainties—is the general standard that the models should be required to meet.

21.2 The models by necessity must be derived using data from tests conducted for durations of time that are very short compared to the very long time scale for application of the models. The type of model validation wherein the material response is measured over the full range of expected in-service conditions is obviously impossible when one of these key conditions is the geologic-scale time of exposure. Unavoidable uncertainties (see Section 24) in time-dependencies within the model can make such long-term projections very difficult, or impossible, to fully validate. However, many material behavior properties do not depend on time. Instead, they depend on environmental conditions (for example, temperature and pH) that may change over time in the disposal system, but over known ranges. That is, for some processes, the values of environmental variables depend on time but the dependence of the material response does not. For these processes, the validity of the model over the range of environmental conditions anticipated to occur over the long service life of the disposal system can be established by using short-term tests that cover the full range of such conditions. Confidence in the validation of the models in this way is usually higher if the models are mechanistic than if they are empirical because of the greater confidence in the relationship between the variables and the response. For example, the dissolution rate of borosilicate glasses depends on temperature, pH, and the activity of dissolved silica. Tests can be conducted over the full range of temperatures, pH values, and silica concentrations (up to saturation concentrations) for direct comparison of the glass dissolution rate with model predictions under the same conditions.

21.3 Some materials behavior models may be partially validated through the use of natural analogs. For example, an alteration model for the degradation of commercial spent fuel might be based on test data in which mineral phases formed as a result of the dissolution of uranium dioxide. The composition of these phases can then be compared to the known composition of mineral phases known to occur in the repository environment over thousands of years to validate the aspect of the model addressing alteration phases. The model cannot be regarded as fully validated, however, because the naturally occurring uranium phases did not evolve in close proximity with other materials that will be present in the EBS, such as zirconium cladding and stainless steel containment materials.

21.4 Some materials behavior models could be partially validated through the use of accelerated tests. For example, a waste container material could be exposed to water or water vapor at a higher temperature than the anticipated in-service condition. The corrosion product resulting from the test could then be compared to that predicted by the model for in-service conditions, and, if similar, could be used to partially validate the corrosion model for the long-term repository conditions.

21.5 In cases where there is insufficient independent data or analyses to adequately support validation of a materials behavior model, a bounding analysis can be used to partially validate the model. A model that can be shown to bound the rate of alteration under all credible environmental conditions may be regarded as validated for the purposes of its usage, which would generally be a conservative over-prediction of the rate of alteration. The bounding model could be mechanistic, semi-empirical, or empirical with regard to the process being bounded.

21.5.1 An alternative approach would be to perform analyses that show there is an upper bound to the amount of alteration due to limits imposed by the mode of alteration. If this is the case, then a constant value could be used for the alteration rather than a model that depends on the values of environmental variables. For example, the near-field temperature in the repository will eventually decrease as a function of time. If the bounding temperature is chosen to be the maximum temperature, then the need to model the variability of the process with temperature might be eliminated. This option is applicable only if the bounding values used for the relevant parameters can be justified. For example, if at some maximum temperature a reaction product is formed that retards the alteration process, but at a lower temperature the reaction product is not formed and the process is not retarded, then use of the maximum temperature might not yield the bounding degree of alteration and is therefore not a justifiable bounding value. A thorough evaluation of the bounding conditions chosen, and the effect of these conditions on the reaction process, should be conducted before the use of the bounding condition.

21.6 It should be recognized that models are essentially simplified representations of actual alteration processes. Models developed under the foregoing procedures may always be superseded by better models. A failure of validation can occur regardless of whether or not a new model gives results that conflict with the results obtained from the initial model. When the new model is proposed, it must be validated by comparing model predictions with test data.

NOTE 2—Validation and confirmation of the model should include independent assessment as supported by testing (characterization, accelerated, service condition, or analog tests, or a combination thereof) and peer review conducted by independent individuals with appropriate backgrounds and experience. Independence is defined by the NRC General Technical Position.[7]

21.7 If the model does not demonstrate the self-consistency of data and is not suitable for the prediction of long-term behavior (see 19.1), it may be necessary to return to the Problem Definition stage (see Section 9). If no alternative models can be conceptualized, it may be necessary to exit the process and select another course of action. Such options are outside the scope of this practice.

PREDICTION

22. Scope

22.1 This element describes the recommended procedure for using validated models to generate predictions of materials behavior for performance assessment purposes.

22.1.1 For each material of interest, the model is used to generate predictions at several stages in the logic shown in Fig. 1. It is useful to differentiate between the two distinct purposes of these predictions: model predictions and repository service predictions.

22.2 Predictions over repository-relevant time scales using the models involve calculations over much longer time periods than can be validated by testing these models. In some cases (for example, corrosion of stainless steels) predictions of

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[7] Nuclear Regulatory Commission General Technical Position, *NUREG/1297*, "Peer Review for High-Level Nuclear Waste Repositories."

repository performance will have to be made by extrapolation of available data using materials behavior models for which considerable mechanistic understanding of alteration behavior may not exist for the environments in question.

22.2.1 If appropriate analogs are available, however, the models are used to interpolate between existing data in order to predict the materials behavior. Since precise matches of analog compositions are unlikely, models must also serve to extrapolate or, preferably, interpolate data against material composition in these instances. The intent of using analog materials (Figs. 1 and 2) is to increase the confidence in the predictions; the models used for extrapolation or interpolation should both adequately represent available data and capture the extent of mechanistic understanding of alteration processes for each material. However, further confidence is afforded the predictions when they are based on interpolations of available data.

22.3 *Prediction Time*—Repository system performance requirements require predictions to be made for events that have at least one chance in 10 000 of occurring within the regulatory compliance period.

22.3.1 For models in which time is not an independent variable, the effect of time on material alteration behavior will occur through changes in the environmental conditions that are variables in the model, such as temperature, pH, solution chemistry, etc.

22.3.2 Modelling may also require the evaluation of possible interactions between the alteration processes of the various materials in the repository system. Some of these effects may be taken into account through variables that are included in behavior models of the individual materials while other effects may require additional variables be taken into account. For example, the dissolution of high-level waste glass will likely increase the pH of the groundwater contacting the steel waste package components to value higher than expected for local groundwater. If the model for steel degradation has a pH-dependence, then the range of pH values for which the steel degradation model is validated should include the pH values expected due to glass degradation.

22.3.2.1 Reactions between the materials of the EBS and the ground water would continue to be important beyond the containment period because the resulting modification of the ground water composition may affect the alteration of spent fuel and glass.

23. Repository Scenarios

23.1 It is recognized that environmental conditions to which materials will be exposed in the repository may change with time after emplacement. Several repository "scenarios," each with some associated probability of occurrence, might need to be considered. For some behavior models, the change in the environmental conditions will be the primary effect of time on material alteration. Predictions generated from most materials behavior models will depend on the particular scenario that is assumed, since most models will have dependencies on temperature, groundwater chemistry, etc. Materials behavior predictions should be generated for each possible scenario. Methods for combining scenarios are considered to be part of performance assessment and are outside the scope of this practice.

23.2 For each scenario, the time dependence of the environmental variables, for example, temperature, groundwater composition, humidity, etc. are expressed as functions of time for use as input variables for materials behavior models in order to generate predictions. Whether or not these are variables in a model is determined during development of the model. The point should be to determine the time dependence of the conditions.

23.3 Particular attention should be paid to mutually exclusive repository conditions to avoid unrealistic scenarios. For example, materials alteration may be rapid if both high temperature and liquid water are present. However, if the repository is porous and thus incapable of maintaining pressurization, these two elements are mutually exclusive.

24. Uncertainties in Model Predictions

24.1 *General Treatment of Uncertainties*—There will be inherent uncertainties in characterizing and modeling the long-term behavior of the waste forms and the materials that provide barriers to radionuclide release. Estimating the reliability and level of confidence that can be attached to the predictions of the long-term behavior for these materials involves identification of the sources of uncertainties for each alteration model. Quantification of these uncertainties is important for those models that significantly contribute to the cumulative uncertainty in the final predictions. This could be done, for example, by performing sensitivity analyses in which ranges of materials alteration model parameter values are used to quantify the impact of hypothetical model uncertainties on the overall performance evaluation. The actual model uncertainties, if known, could than be statistically propagated through the overall material behavior evaluation to arrive at quantitative estimates of uncertainties in the predictions. The capability of individual materials alteration models to provide reliable predictions of materials behavior over long time periods will be strongly dependent on the sources of uncertainties in those models. Model uncertainty can result from mathematical model uncertainty and conceptual model uncertainty. Mathematical model uncertainty arises from the simplifying assumptions and approximations used in formulating the mathematical form of the model. Conceptual model uncertainty arises from the incomplete understanding of the mechanisms that dominate the material behavior. The uncertainties that require consideration may include:

24.1.1 The mathematical form of the model itself (for example, have appropriate mathematical functions been selected to model the processes?),

24.1.2 The effects of key alteration modes in the model,

24.1.3 Materials interaction effects,

24.1.4 The test data used to determine parameter values, and

24.1.5 The predicted environmental service conditions.

24.2 *Uncertainty in the Mathematical Form of the Model*—[addresses PA requirement in 10 CFR 63.114 (c)]— Uncertainty in the analytical form of an alteration model itself is perhaps the most difficult source of uncertainty to quantify adequately. The primary source of uncertainty in the prediction of a particular mode of materials alteration over the very long repository-relevant time periods is likely the mathematical form of the model. This source of uncertainty would likely decrease as models become more mechanistic as opposed to empirical. Models that mathematically represent actual physical or chemical processes of materials alteration operative over the time period the model is applied have less inherent uncertainty. Fully empirical models may be used as bounding cases, or when mechanistic models are not available or practically achievable, but the predictions of these models are considered to have greater uncertainty. For example, a bounding empirical model based on some high multiple of an actually observed alteration rate could be used as part of a highly conservative analysis of EBS performance with high confidence, but the confidence in the accuracy of the level of alteration predicted by the model would be very low.

24.3 *Test Data Uncertainty*—[addresses PA requirement in 10 CFR 63.114 (g)]—Most data used to develop models will have been obtained over short periods of time compared with the repository-relevant time periods. Additionally, any test data used to support model development will have associated with them accuracy and reproducibility limitations that must be factored into any model derived from the data. This source of uncertainty may be mitigated by the use of data from accelerated tests, and to the extent that there is a mechanistic basis for using the model to predict long-term alteration.

24.3.1 *Fitting Parameter Uncertainty*—[addresses PA requirement in 10 CFR 63.114 (b)]—Model fitting parameters are values assigned to coefficients used in a materials alteration model, and are generally obtained from test data using curve-fitting or data regression techniques. Alternatively, parameter values may be based on theory, data from the open literature, expert judgment or some combination thereof, each of which has its associated uncertainty. But this uncertainty can be further minimized to the extent that the alteration mechanisms are understood and incorporated into the form of the predictive models. Model fitting parameters should not imply a degree of accuracy in the application of the alteration model that exceeds the accuracy of the test data used to derive the fitting parameters. For example, if corrosion rate data with an experimental accuracy of ±10 % were regressed using a model similar to that of Eq 5, the "k" fitting parameter should not be expressed to more than two significant figures. The uncertainty in the fitting parameters should reflect the uncertainty in the data used to derive them.

24.3.2 *Propagation of Data Uncertainties*—Uncertainties in the data and parameters on which the materials behavior models are based should be propagated through the model to obtain their contribution to the overall uncertainty in the predictions by using appropriate statistical techniques.

24.4 *Uncertainties in Establishing Environmental Service Conditions*—[addresses PA requirement in 10 CFR 63.114 (a)]—Uncertainties in establishing the environmental conditions to which materials will be exposed—including the evolution of those conditions with time and materials interactions—should be evaluated for their contribution to the uncertainty in the final materials behavior predictions. The prediction of the evolution of the physical/chemical environment to which the EBS materials will be exposed over the very long service time is beyond the scope of this standard, but should be expected to contribute additional uncertainties.

24.5 *Confidence in Materials Alteration Predictions*—Predictions from models of materials behavior over short periods are expected to have intrinsically high confidence levels, since even fully empirical models must be validated to reproduce alteration levels that have been already directly observed. Predictions for longer periods of time are expected to have lower confidence levels and will require achieving reasonable assurance as defined in the NRC regulations [see 10 CFR 63.101(a)(2)]. However, confidence levels will also depend on the particular repository scenario under consideration and the selection and identification of WP/EBS materials.. For example, when a dry environment is expected due to high-level waste decay heat, the prediction of low rates of alteration processes would have relatively high confidence levels.

24.5.1 The selection of EBS barrier materials could be influenced by the level of confidence in the model for the expected .primary degradation mode/mechanism. The degradation model for a less corrosion resistant material may have a sufficiently higher level of confidence than that of more highly corrosion-resistant candidate materials, and the higher rate of degradation expected for the alternative material may be compensated by the consequent greater model confidence and, for example, by incorporating a "corrosion allowance" into the barrier design.

24.6 *Confidence with Respect to Excluded Alteration Modes/Mechanisms*—[addresses PA requirements in 10 CFR 63.114 (e) and (f)]—The high level nuclear waste to be disposed in the repository may consist of many (~250) different types of waste forms; several kinds of commercial light water reactor spent fuel assemblies, high level radioactive waste glass logs, immobilized Pu ceramics, and several hundred distinct forms of non-commercial and test reactor spent fuels. It is not practical to obtain waste form-specific alteration models for all waste form types. It is expected that, in many cases, the alteration mechanisms for a waste form B will be similar enough to that of another waste form A that has undergone appropriate testing that the alteration model determined for waste form A may also be applied to waste form B. However, it is possible that an alteration mechanism that was not observed in the testing of waste form A could significantly contribute to alteration of waste form B under long-term repository conditions. Since they are not modeled, the contributions of such mechanisms to materials performance uncertainty is not taken into account. An emphasis on the mechanistic understanding of potential alteration modes, careful selection of representative materials for testing, and appropriate Characterization and Accelerated tests should minimize the probability that a significant mode of alteration will be overlooked or unduly discounted when developing the alteration models. The statutorily required Confirmation testing (see below) would also add to the confidence that no reasonably probable alteration mode has been overlooked.

PERFORMANCE CONFIRMATION

25. Scope

25.1 *Performance Confirmation Requirements*—During the pre-closure or operational period for a geologic repository (approximately 70 or more years), it is expected that additional data concerning the long term behavior of EBS materials will have been accumulated through confirmation testing, The requirements for confirmation testing are described in Subpart F, "Performance Confirmation Program," of 10 CFR Part 63.102(m), 63.131 and 63.134 . These tests, referred to in this practice as confirmation tests, are intended to provide further confirmation of the validity of the model. The confirmation tests will provide additional testing data to which the model predictions can be compared. Confirmation testing should focus on the alteration modes of those EBS and waste form materials that are most likely to impact the overall repository performance. These key alteration modes can be identified through performance assessment sensitivity analyses, expert judgment, analysis of natural analog materials, etc. Identification of such key alteration modes should take into account the inventory of spent fuel or high level waste to be emplaced as well as the expected rate of alteration of that waste in order to account for boundary dose risk.

25.2 *Performance Confirmation Testing*—Performance confirmation encompasses a continuous, broad-based, technical program of tests, experiments, and analyses, conducted to provide the information needed to confirm the design and performance of the repository system through construction and operation to permanent closure. Subpart F 10 CFR Part 63.131(2)(b) requires establishment of the performance confirmation program during site characterization and to continue the program until permanent closure. An appropriate performance confirmation program should provide information necessary to determine with reasonable assurance whether the Yucca Mountain repository can be safely closed. Subpart F 10 CFR Part 63.134 "Monitoring and Testing Waste Packages" requires that:

25.2.1 A program should be established at the geologic repository operations area for monitoring the condition of the waste packages. Waste packages, and the waste forms they contain, chosen for the confirmation test program should be representative of those to be emplaced in the underground facility.

25.2.2 Consistent with safe operation at the geologic repository operations area, the environment of the waste packages selected for the waste package monitoring program (WPMP) should be representative of the post-closure environment in which the wastes are to be emplaced.

25.2.3 The WPMP should include laboratory experiments that focus on the internal condition of the waste packages. To the extent practical the environment experienced by the emplaced waste packages within the underground facility during the WPMP shall be duplicated in the laboratory experiments.

25.2.4 The WPMP shall continue as long as practical up to the time of permanent closure.

26. Specific Procedure

26.1 Identify processes and parameters that are important to post-closure performance. Identification should be made based on a risk-informed performance-based (RIPB) approach. RIPB focuses on tests, experiments, and analyses that address Features, Events, and Processes (FEPs) for which the projections of long-term repository performance are particularly sensitive, and which have a significant degree of uncertainty in meeting regulatory requirements.

26.2 Select processes and associated parameters that require performance confirmation testing using RIPB approach.

26.3 Analyze existing data and models to establish tolerances or predicted limits or deviations from predicted values for key parameters of the selected processes.

26.4 Identify completion criteria and guidelines for corrective actions to be applied when variances occur.

26.5 Conduct detailed planning of test and monitoring activities to measure key parameters.

26.6 Monitor performance, perform tests, and collect data.

26.7 Analyze and evaluate the collected data using process models, statistical tests, and total system performance assessments.

26.8 Recommend and implement appropriate actions if data is outside the established tolerances or predicted limits or deviates from predicted values of the parameters.

27. Quality Assurance

27.1 This practice covers "activities related (to the) design and characterization of barriers important to waste isolation" and that are accordingly subject to the quality assurance requirements in 10 CFR Part 63 (Subpart G).

27.2 All data collection and predictive modeling shall be done under a qualified Quality Assurance Program (such as NQA-1). The QAP will assure that the quality assurance requirements of 10 CFR Part 63 (Subpart G) are met.

27.2.1 DOE Nuclear Quality Assurance for High Level Radioactive Waste Management is embodied in DOE/RW 0333P, and is the preferred standard for a comprehensive quality assurance guide. Other consensus standards such as ANSI NQA-1, ASTM standards, the International Organization for Standardization (ISO), and other standards should be used as guidance or references.

27.3 Acceptable data must be recoverable, defensible, and traceable.

27.3.1 Data are recoverable when they are completely documented in accessible records.

27.3.2 Data are defensible when they have been obtained by documented and approved test methods using good laboratory and field test practices and are reproducible.

27.3.3 Data are traceable when they can be related through an unbroken chain to acceptable reference standards, calibration checks, and parallel experiments using standard reference materials from authoritative sources such as National Institute of Standards and Technology, United States Geological Survey, Environmental Protection Agency, or a U.S. Department of Energy-approved source.

27.4 Predictive models in the form of computer software must be fully documented as required by NUREG-0856 and a software quality assurance plan approved under the QAP governing the activity. Note that NUREG-0856 requires: a theoretical manual, a users manual, copies of the source code on magnetic media, paper hard copies of the source code, a summary of the software, and an assessment of the code with supporting programs and documents.

28. Precision and Bias

28.1 The parameter values in the alteration models developed under this practice, when determined using curve-fitting and regression of experimental data from accelerated, characterization, and service condition tests, should reflect the precision and bias limitations of that data. The accuracy of a materials alteration model should not be taken as greater than the precision of the test data from which the model and model parameters are derived. Statements of precision and bias should be developed for the test data used to support model development and the consequent quantitative predictions resulting from the application of this practice. (See Practices E 177, E 178, and E 583).

28.2 The factors that contributed to the uncertainty in the predictions should be described and the significance of their contribution described and, when possible, quantified.

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