Designation: C 1174 – 97

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 covers steps for the development of methods to aid in 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 high-level nuclear waste in the U.S. Government disposal site.

1.1.1 These steps include problem definition, testing, modeling, and confirmation.

1.1.2 The predictions are based on models derived from interpretation of data obtained from tests and appropriate analogs.

1.1.3 These tests may include but are not limited to the following:

1.1.3.1 Attribute tests,

1.1.3.2 Characterization tests,

1.1.3.3 Accelerated tests,

1.1.3.4 Service condition tests,

1.1.3.5 Analog tests, and

1.1.3.6 Confirmation tests.

1.1.4 Tests performed on analog materials.

1.2 The purpose of this practice is to provide information to serve as part of the basis for performance assessment of a geologic repository.

1.3 This practice does not cover other methods of making predictions such as use of expert judgment.

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 limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*

E 177 Practice for Use of the Terms Precision and Bias in ASTM Test Methods[2]

E 178 Practice for Dealing with Outlying Observations[2]

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]

ANSI Nuclear Quality Assurance for Waste Management

ANSI/ASME NQR-1 Quality Assurance Program Requirements for Nuclear Facilities

2.3 *U.S. Government Documents:*

DOE/RW-0333P, Rev. 7, Quality Assurance Requirements and Description, USDOE OCRWM, Oct. 1995

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

Materials Characterization Center Guidelines for Accuracy and Precision of Test Data. In Nuclear Waste Materials Handbook-Volume on Test Methods. U.S. Department of Energy, DOE/TIC-11400[6]

Public Law 97-425, Nuclear Waste Policy Act of 1982, as amended[7]

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

3. Terminology

3.1 *Definitions*:

3.1.1 Definitions used in this practice are existing ASTM definitions,[8] when applicable.

3.1.1.1 Definitions of some terms "specific to this practice" are based on the referenced Code of Federal Regulations, 10

[1] This practice is under the jurisdiction of ASTM Committee C–26 on Nuclear Fuel Cycle and is the direct responsibility of Subcommittee C26.13 on Repository Waste Package Materials Testing.

Current edition approved December 10, 1997. Published August 1998. Previously published as C 1174 – 91. Last previous edition C 1174 – 91.

[2] *Annual Book of ASTM Standards*, Vol 14.02.

[3] *Annual Book of ASTM Standards*, Vol 12.02.

[4] Available from American National Standards Institute, 11 W. 42nd St., 13th Floor, New York, NY 10036.

[5] Available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20402.

[6] Available from the National Technical Information Service, U.S. Department of Commerce, Springfield, VA 22161.

[7] In "United States Statutes at Large," available from Superintendent of Documents, U.S. Government Printing Office, Washington, DC 20002.

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

CFR Part 60,[9] 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.

3.1.1.2 For any other use of the terms in this practice consider carefully the context in which they are defined here.

3.1.2 *Regulatory and Other Published Definitions*:

3.1.2.1 *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.

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

3.1.2.3 *Geologic repository*—a system which is intended to be used for, or may used for, the disposal of radioactive wastes in excavated geologic media. A geologic repository includes:" (1) The geologic repository operations area, and (2) the portion of the geologic setting that provides isolation of the radioactive waste.

3.1.2.4 *high-level radioactive waste*—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.

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

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

3.2 *Definitions of Terms Specific to This Standard:*

3.2.1 *accelerated test*—a test that results in an increase in the rate of an alteration mode, when compared with the rates for service conditions. Changes in alteration mechanism, if any, must be accounted for in the use of the accelerated test data.

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

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

3.2.4 *alteration mode*—a particular form of alteration, for example, general corrosion, passivation.

3.2.5 *analog*—a material whose composition, and environmental history are similar enough to those of the materials of interest to permit use of conclusions about it to be applied to the materials of interest. Alternatively, a process that is similar enough to the process of interest to be used in this manner.

3.2.6 *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 repository environment. Examples are thermal conductivity, mechanical properties, radionuclide content of waste forms, etc.

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

3.2.8 *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.

3.2.9 *characterization test*—in high-level radioactive waste management, any test conducted principally to furnish information for a mechanistic understanding of alteration. Examples include polarization tests, potential-pH (Pourbaix) diagrams, solubility analyses, and x-ray diffraction of corrosion layers.

3.2.10 *confirmation test*—a test whose results had not been used in the validation of a model but are available and used later to further validate its predictions. Under current regulations, these tests can be conducted over much longer periods of time than that available (in the pre-licensing phase of the process) for validation tests.

3.2.11 *degradation*—any change in the properties of a material that adversely affects the behavior of that material; adverse alteration.

3.2.12 *empirical model*—a model based only on observations or data from experiments, without regard to mechanism or theory.

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

3.2.14 *model*—a simplified representation of a system or phenomenon, along with any hypotheses required to describe the system or explain the phenomenon, often mathematically.

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

3.2.16 *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.

3.2.17 *semi-empirical model*—a model based partially on one or more mechanisms and partially on data from experiments.

3.2.18 *service condition test*—a test, of a material, conducted under conditions in which the values of the independent variables characterizing the service environment are in the range expected in actual service.

3.2.19 *model validation*—the process through which independent measurements are used to ensure that a model accurately predicts an alteration behavior of waste-package materials under a given set of environmental conditions (e.g. under repository environment over the time periods required).

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 and validation of appropriate models, to formulation and confirmation of actual predictions.

5. Significance and Use

5.1 This practice is intended to guide in making predictions of alterations in materials over periods of time beyond which empirical data can be used for the accurate assessment of performance and behavior. Under very extended service periods, much greater than the periods encountered in engineering

[9] An alternate to this practice's recommendation (to demonstrate one or more alteration mechanisms that apply to a behavior model) is the development of predictions based on the long–term approach to thermodynamic equilibrium (or steady-state) behavior.

practice, materials may become altered and may change in form or state. The time period, when sufficiently long, can even permit the achievement of equilibrium or steady state conditions and render kinetic factors, which govern rates of reactions, to be much less important. This practice is intended for use specifically for materials proposed for use in an EBS that contains high-level nuclear waste. These packages are to be emplaced in deep geologic repositories in which retrieval after closure is not contemplated – cf. 10.2 on scope of testing. 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. Licensing of such disposal will be done by the U.S. Nuclear Regulatory Commission (NRC).

5.1.2 The NRC regulations in Part 60.113 of Title 10 of the Code of Federal Regulations (CFR) provide that containment of radionuclides shall be substantially complete for a period that shall be no less than 300 years nor more than 1000 years, unless otherwise permitted by the NRC. Any release of radionuclides after the containment period shall be a gradual release and limited to certain small fractional amounts based on the calculated inventory present at 1000 years after closure. These are general provisions, for the EBS, for which only anticipated processes and events need to be considered.

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 10 000 years 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. Analyses of overall repository system performance may include anticipated and unanticipated events.

5.2 Regulations that are site specific, i.e., applicable to a particular site may be required to be developed in the future; current (cited) regulations apply to any repository in the United States—cf. 8.2 conceptual design.

5.3 It is recognized that data on the actual long-term behavior of any materials used in the EBS and exposed to repository conditions for such long periods of time will not be available for use in the design of waste packages.

5.4 This practice is intended to meet the need for defining acceptable methods for making useful predictions of long–term behavior of materials from such sources as data and analogs.

5.5 The EBS environment of interest is that defined by the natural conditions (e.g. minerals, moisture, biota, and stresses) as modified by effects of time and repository construction, and operations, and the consequences of the radionuclide decay, e.g. radiation, heat. The conditions associated with both anticipated and unanticipated scenarios are to be considered.

6. General Procedure

6.1 Fig. 1 outlines the logical approach for the development of models for the prediction of the long-term behavior of materials within the EBS of 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 a given plan will contain all of the elements described, as well as a quality assurance program as discussed in Section 27 Details on these elements are given in Sections 7-26.

PROBLEM DEFINITION

7. Scope

7.1 Important to predictions of long-term behavior of repository materials are the following: the identification of environmental conditions; waste-package concepts: candidate materials for waste packages; the form of the waste; alteration modes, analog materials; and literature surveys.

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

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

8. General

8.1 *Site Characterization*—A proposed repository site is characterized, in a preliminary manner, with respect to the geology, hydrology, etc. For purposes of this practice, site characterization is done to identify likely environmental conditions associated with the repository site (see 8.5.1, 9.1, and 10.2).

8.1.1 *Environment*—The geologic environment of the EBS shall be initially identified by characterizations of both the environment and extant understanding of the effects of time on the environment. Ranges in the values of environmental parameters may be required, so as to accommodate uncertainties in estimates of their values and to account for environmental conditions, such as climate, that may change over time.

8.2 *Conceptual Designs*—A general concept for an EBS is devised to meet regulatory requirements—cf. 5.1.4 for regulatory perspective. Specific designs for the components of the EBS are developed based on current understanding of the conditions of a particular site.

8.3 *Materials*—From the initial concepts and investigations of a repository site, candidate materials are proposed based on the geologic environment and the conceptual design. Since these materials serve the function of containment and control of potential release rates, their long-term behavior under the set of conditions expected in the repository over long time periods

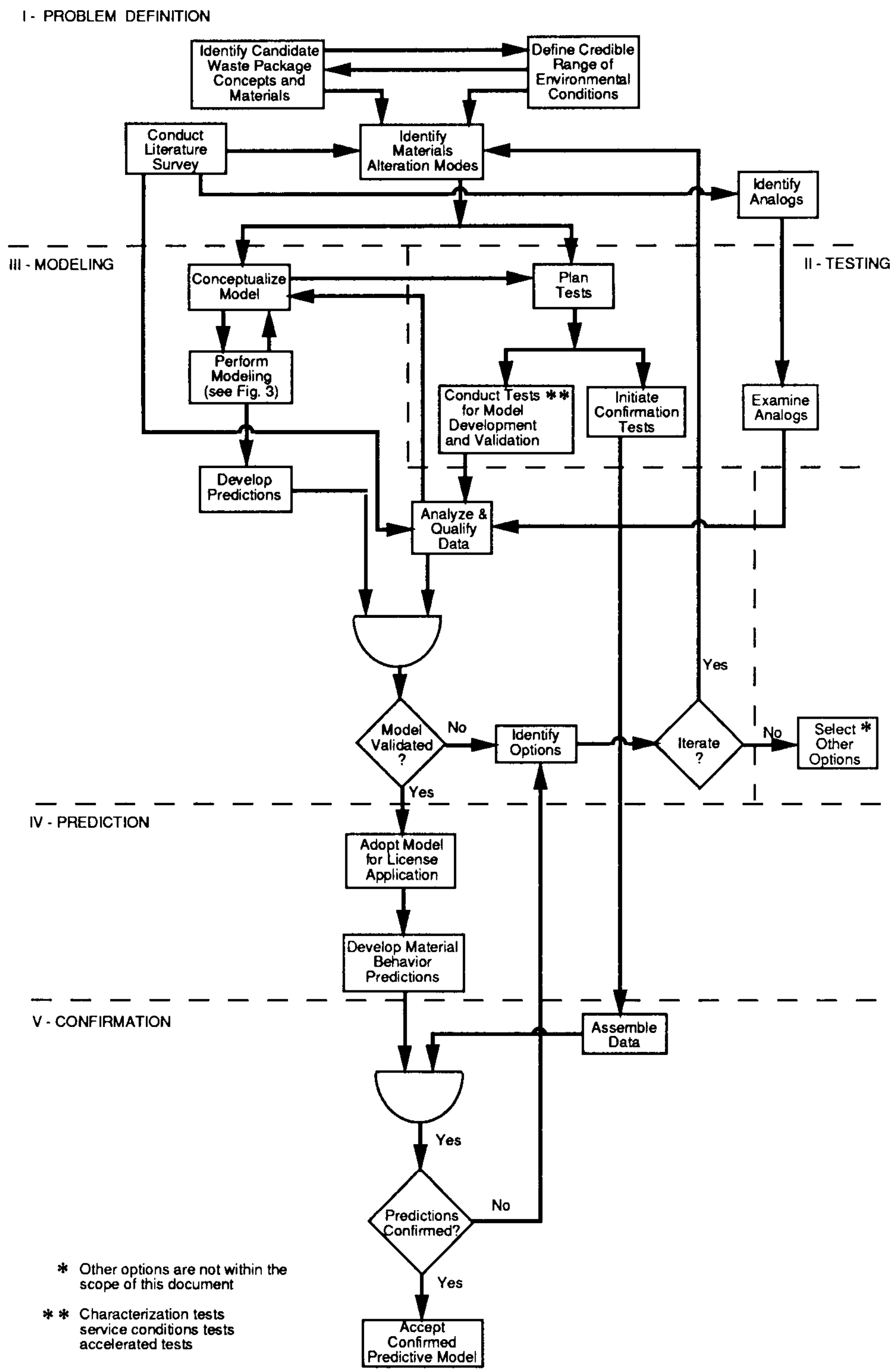

FIG. 1 Logic for the Development of Predictive Models for the Post-Closure Behavior of Waste Package Materials

must be established, and the alteration modes for these materials must be clearly understood. This understanding is developed by first reviewing both the available information on the environmental conditions and the effects of these conditions on the candidate materials.

8.3.1 Information on natural analogs might be available to provide early guidance on the materials selection process.

8.4 *Data Ranges*—Preliminary descriptions of the materials to be tested shall be used to characterize their physical and mechanical properties. Frequently, a range may be needed to specify parameters used to characterize materials.

8.4.1 A range of environmental conditions or material properties may be used for various reasons: uncertainty in a measurement, variabilities in production or in nature, etc. The waste forms themselves may have to be described by ranges. Neither vitrified waste nor spent fuel will likely lend themselves to precise descriptions without the use of range information. For example, variations in production history, product usage, and process control will affect important properties of waste forms. In addition, over long times, some properties of waste forms will change.

8.4.2 *Bounding conditions*—Bounding conditions furnish necessary input to bounding models which may be useful in making predictions of performance limits. It is noted that before the use of bounding conditions, thorough evaluations are generally required of the alteration mechanisms, all important parameters, and the effects of each parameter on the anticipated alteration processes. When ranges are needed to specify values either for materials or for environmental conditions, bounding conditions should be based on the extreme credible values for these variables.

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 the testing stage of this practice. Before the collection of that data is regarded to be complete, various preliminary modeling and testing efforts can be initiated and even completed, so as to expedite the processes of understanding the material/environment system and of making confirmed predictions of the alterations that will occur over extended times in a repository.

8.5.1 *Interactions*—The process of predicting metals behavior in repositories must involve consideration of interactions between materials and complex environments. For example, interactions between various materials and the environment lead to the formation of reaction products that, in turn, become part of the environment. Microbes, seismic events, etc., make the environment more complex and should 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 identify possible alteration modes. A literature survey must be conducted to evaluate any analogs that are to be used in later validation activities.

8.7 *Preliminary Models*—For each important alteration process, preliminary models shall be developed to represent processes, postulates, and inferences related to observed and expected behavior of the materials in the proposed containment system.

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

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

9.1 *Environmental Conditions*—Determine the environmental conditions to which the material will be exposed after emplacement. Many of these conditions are, of course, site specific. For example, ground-water composition, may be affected as material degradation occurs throughout the repository. The extent of such secondary interactions may be difficult to quantify initially, but must be noted and accounted for in the 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 identify modes for the materials of interest, using environmental conditions that are appropriate for the specific proposed repository being evaluated.

9.5 *Variables*—Identify the variables regarded to be important to performance, as for example, the amount of water that is expected to contact a waste glass. For each independent variable, attempt to identify the expected range of values. Consider whether the number of variables and the range can be decreased by elimination of those that do not significantly affect behavior of materials.

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 more 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. These may be either natural or historic.

9.7.1 Identify the aspect of the analog that can be compared with the material under consideration. Differences will exist between the compositions (or the environments) of the analog and the repository material. Evaluations of the significance of the differences may be used to support or disqualify the analog as a means for validation of the alteration model.

TESTING

10. Scope

10.1 Testing of EBS material is required to establish whether candidate materials meet the regulatory requirements, e.g. those on containment and control of release rates in 10 CFR Part 60. Tests conducted over a comparatively short period, e.g., 10 to 20 years, will be used to support development of predictive behavior models for the response of the materials to the repository environment over time periods up to 10,000 years. The testing program will 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 minimization of 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 early testing concepts described herein do not specifically address the testing of integrated systems of the EBS. These 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, (groundwater quantity, groundwater chemistry, host rock properties, etc.) but it could be used for host rock or for any component material, to predict the behavior of that component.

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 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 that could occur in the repository environment after long periods of time. For example, a simulation could be 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 Provide 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

11.1 *Types of Tests*—The tests listed in 1.1.3 are described here. Fig. 1 shows the relationships among them. A single test could simultaneously serve more than one of the stated functions. For instance, a single test procedure could serve as both a characterization test and as an accelerated test. 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 of materials properties and characteristics, like grain size, hardness, or tensile strength.

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

11.1.2.1 Service condition tests provide an alteration data base for "initial conditions."

11.1.2.2 Characterization tests are designed to establish alteration mechanisms.

11.1.2.3 Accelerated tests are designed to produce, over a short time period, alterations that simulate the long term.

11.1.3 *Confirmation Tests*—These tests are expected to be conducted over extended times and they are intended to provide further assurance as to the validity of predictions of long-term behavior. The predictions are made from the models developed and validated by the procedures of this practice.

11.2 *Behavior Model*—The alteration of an EBS material can be predicted from a behavior model, which is developed from characterization tests, accelerated tests, literature analyses, and analyses of analogs. The model is fitted using a combination of results from these tests and date from service-condition-tests.[9]

11.2.1 The form (Arrhenius, constant rate, etc.) of the behavior model reflects (and, to some extent, governs) the nature of the testing used to validate it. For example, an alteration mode having an Arrhenius form may require that tests be conducted over a particular range of temperatures over carefully selected intervals.

11.2.2 The ability of the behavior model to provide reliable predictions will be strongly dependent on the uncertainties in the model itself, the test data used to calibrate the model, and the actual in-service boundary conditions (see Section 24 on Uncertainties). The statistical analysis of these uncertainties may aid in the evaluation of test data.

11.2.3 The reliability of model predictions will depend upon how well the model represents, over time, both the mechanism of in-service alteration behavior (e.g., type or stoichiometry of corrosion product, form of alteration layers, mode of degradation) and the in-service environmental conditions (e.g., temperature, groundwater chemistry, groundwater quantity).

11.2.4 The closer the model simulates the actual physical and chemical alteration (that is, the more mechanistically based the model is), the lower the intrinsic uncertainty in the predictions will be.

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. There is no need to model the time dependence of these properties. These properties are input to the behavior models.

12.1.1 Examples of such properties are thermal conductivity, chemical composition, radionuclide content of the waste forms, mechanical properties of candidate container materials, 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 or correlations are not available from 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 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 process of material alteration expected in the repository environment. These 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 (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 is necessary to investigate the sensitivity of the alteration mechanisms to variations in the values of particular parameters, so that appropriate values can be used.

13.1.2.1 Examples of these tests include anodic polarization tests, potential–pH (Pourbax) diagrams, radionuclide solubility analyses, x–ray diffraction analyses of corrosion or alteration layers, etc.

13.2 *Specific Procedure-Characterization Tests*:

13.2.1 Identify the candidate EBS material and the credible range of repository-relevant 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, without changing the alteration mechanism(s) associated with the alteration mode under investigation. Therefore, knowledge of the mechanism is needed for the design of the accelerated test and meaningful use of accelerated test data.

14.1.1 If, during an accelerated test, the alteration mechanism changes or does not conform to that assumed in the behavior model, either the model must be reformulated to reflect the change in mechanism, or the accelerated test conditions must be re-evaluated for their relevance to the repository condition.

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 use the B rate data in the rate model for *A*. If *B* is judged to be due to a possible 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 alter the state of a material in a short time to simulate long time repository exposures, and there by 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.

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 must be quantified and mechanically described.

14.1.3 *Synergisms*—Because of the potentially large number of test parameters (for example, temperature, radiation, mechanical stress, groundwater chemistry, and material condition) careful consideration must be given to possible synergistic effects among the test parameters.

14.1.4 *Models*—Results of accelerated tests can be used to develop or validate a behavior model by verifying a null result at extreme conditions, and at another extreme.

14.1.4.1 As an example of a null result, a test for stress corrosion cracking (SCC) of a candidate waste container material might be conducted to establish the bounds of temperature and water chemistry conditions. These might include higher temperatures and more aggressive water chemistry within which a stress corrosion crack would not initiate.

14.1.4.2 For the other extreme, a test for general corrosion may be conducted at higher temperatures 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.

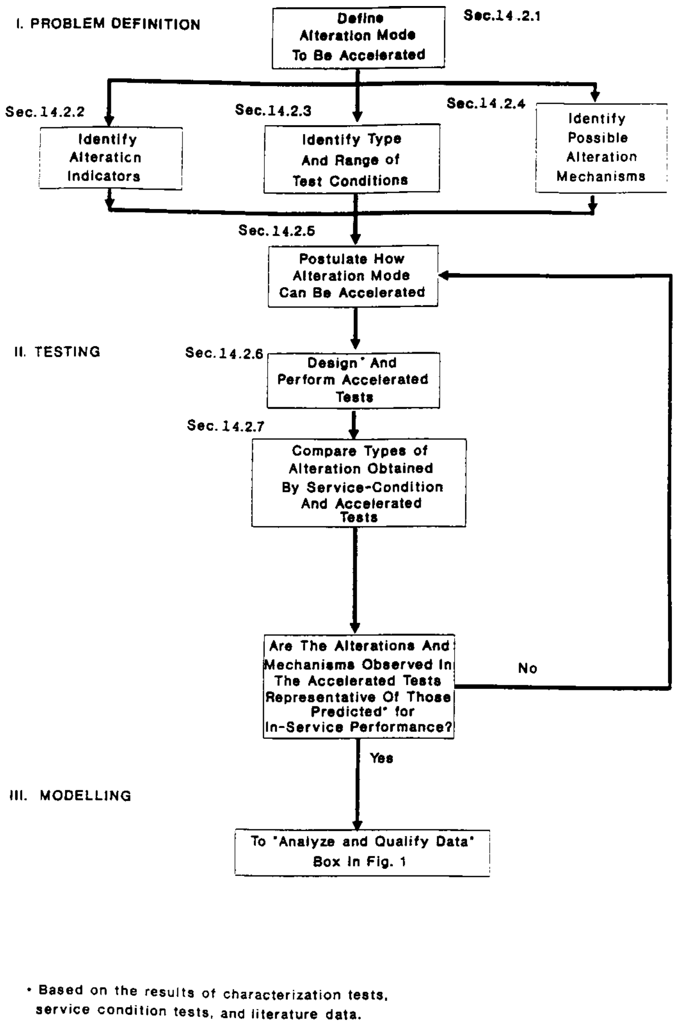

FIG. 2 Recommended Procedure for Developing Accelerated Tests for Waste Package Component Materials

14.2.5 Postulate how the alteration mode can be accelerated.

14.2.6 Perform tests using a prescribed set of parameters, i.e. 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.

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 goal of service condition testing is to establish a suitable data base for determinations of the mechanisms of alteration behaviors of (EBS) materials under repository-relevant conditions.

15.1.1 These tests identify the key parameters (for the materials and the environments) that affect the alteration mechanisms under expected conditions. Observations of the alteration mechanisms under service conditions can then be used as the basis against which the relevance of accelerated test results (and the mechanisms observed therein) can be proven.

15.1.2 Service condition tests should be designed to show the dependence of material behavior on each (and every) relevant environmental condition. Service tests should be conducted over the full expected range of repository conditions for each important factor.

15.1.3 Service condition tests establish reference test conditions that can be used to calibrate or verify test responses for long-term confirmation testing (see Section 13).

15.1.4 Service condition tests provide data on alteration of materials under actual repository test conditions by use of short-term *in-situ* (e.g., in the repository exploratory shaft 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. 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 average or expected 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 reveal the range of responses embraced by the "normal" conditions. Note that the most severe conditions may not be the maximum value for each variable.

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. Accordingly, analogs would be best used 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 is necessary to establish that, in natural and experimental environments, the analogs behave similarly. This supports 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, including:

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 Complete chemical analysis.

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

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.

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.

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 after predictions have been made from a validated model, in order to further validate the model. During the pre-closure period of the repository, testing (particularly *in-situ* testing) should be continued so as to determine key aspects of materials behavior for the EBS. Also, tests that had begun as service condition tests could be extended, so at to serve the purpose of confirming, over the pre-closure period, the material (behavior model) predictions.

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 or verified to be present within the repository. Alternatively, they must be conducted to furnish more details than were possible during the validation phase. For example, by exploring selected parameters for which no data or insufficient data had been made available during 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 validated 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 This element focuses on expressing the data obtained by the various tests in terms of mathematical equations relating the variables that have been found to be significant.

18.2 General considerations in modeling are covered as well as specific procedures.

18.3 It is recognized that development of a mathematical model for the processes under consideration may not be possible in all cases.

19. General

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

19.2 *Types of Data to be Modeled*—This practice provides for the use of several types of information and data:

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 Other literature information.

19.3 *Types of Models*—Quantitative models may range from purely empirical to purely mechanistic.

19.3.1 *Mechanistic:* Purely mechanistic models may be illustrated by reference to Eq 1:

$$Y = F(x_1),\ i = 1 \text{ to } n, \tag{1}$$

where:

$F(x_i)$ represents the dependence of Y, the dependent variable of interest, on the x_i, the n variables that affect Y.

19.3.1.1 Mechanistic relationships may be derived through a series of steps (or reactions) that lead to understanding on postulated interaction between a material and its environment. This series of steps constitutes the proposed mechanism, for the interaction. The relationship derived, through studies of the behavior, is properly considered to be a mechanistic model. In the relationship, everything has been accounted for, including numerical constants, and there are no residual terms–a distinction is made between deficiencies in the model and errors in collecting experimental data. Therefore, predictions made from mechanistic models can be attended by high degrees of confidence.

19.3.2 *Substantial Mechanistic Understanding:* Several deficiencies exist for the mechanistic model. (1) The time required to develop such a model may be impractical. (2) An analytical representation 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, sometimes a purely mechanistic model may be unattainable, especially one that can be used in a practical sense.

19.3.2.1 For the purposes of this practice, however, models in which there is substantial mechanistic understanding of the alteration processes may be considered as mechanistic models. These models may be illustrated by reference to Eq 2:

$$Y = f(x_i) + \epsilon,\ i = 1 \text{ to } n, \tag{2}$$

where:

Y = is the dependent variable of interest,

$f(x_i)$ = is known and based on mechanistic understanding,

ϵ = is a residual not accounted for by $f(x_i)$, and x_i is the ith independent variable.

The approach is to postulate a series of steps or reactions as being representative of the most pertinent processes, even though these may not represent the behavior precisely. One infers, by scientific reasoning, a relation of the form of Eq 2. The objective is to obtain a relation in which the residuals are tolerable or negligible.

19.3.3 Purely empirical models appear frequently in the technical literature.

19.3.3.1 The approach for empirical models is to obtain a relationship that accounts for observed data, within a margin of experimental error. The approach is purely empirical when no "mechanisms" are apparent and postulated. Instead, parameters believed to have an effect on the dependent Y are identified, measured, and correlated with observed values of variable Y. The correlation may be direct, or it may involve dimensional analysis to arrive at groupings that individually have dimensionless numerical values. The independent variables may initially be chosen on the basis of judgment, inconclusive data, or some partially applicable theories. For example, it might be hypothesized that the corrosion rate of a certain steel should be affected by the concentrations of hydroxyl and chloride ions in the water to which it is exposed. A possible conceptual model based on a statistical approach could be as follows:

$$dY/dt = a_0 + a_1x_1 + a_2x_2 + a_{12}x_1x_2 + \epsilon, \tag{3}$$

where:

Y = the extent of an alteration whose change with time depends on the concentrations of x_1(hydroxyl ions) and x_2(chloride ions). The data obtained might permit the following form:

$$dY/dt = a_1[OH-] + a_2[Cl-]. \tag{4}$$

This model supports the conclusion that the interaction term is negotiable. This is an empirical model.

19.3.3.2 The principal difficulty with empirical models is that the applicability of extrapolations usually decreases rapidly the further one extends them beyond the values used for parameters in the original experiments. Thus, for the purposes of this practice, purely empirical models are considered to be unacceptable, as they can not be extrapolated and the data are required for very long times in repository applications.

19.3.4 Semi-empirical models represent a practical compromise between the mechanistic and empirical models. The semi-empirical model incorporates at least some mechanistic understanding into the modeling process. It is valid over a larger range than the purely empirical models provided that a) the mechanisms involved are known to persist over the observed range of time, b) the mechanisms are known to continue to be operable over the time range of the predictions, and c) there is no evidence for other operable mechanisms—those that might begin to operate and dominate the alteration processes.

19.3.4.1 Confidence is greatest at the mechanistic end of this scale of semi-empirical models. Hence, the fewer the number of empirical elements in the models, the greater is the confidence in their application.

19.3.4.2 An example of a semi-empirical model follows: If the Guldberg and Waage Law of Mass Action is invoked in a second-order kinetic equation, the Eq 5 may be written:

$$dY/dt = k[OH-]_{\alpha}[Cl-]_{\beta} \quad (5)$$

This relates a reaction rate to basic parameters of concentration (or more precisely, activity). It is nevertheless empirical because it requires experimental determination of the constants k, α, β. If an expression for *k* could be derived from fundamental principles there would then be a model that approaches the purely mechanistic. However, it still does not describe the exact sequence of steps in the chemical reactions of corrosion.

20. Steps in Modeling

20.1 Modeling is iterative in nature. Fig. 1 shows that the initial iteration involves formulating a conceptual model around which to plan acquisition of test data. These data are used to quantify the model which is then checked for closeness of fit to the actual data. Fig. 3 shows the modeling process in more detail.

20.2 Empirical analysis is usually the initial step because generally the identities of the significant variables are unknown or uncertain. Thus, the available data are analyzed for relationships and trends. Another objective is to look for evidence of changes in alteration mechanisms.

20.3 *Analyze and Qualify Data*—All data used in modelling should be qualified. Ideally, the data are collected in a Quality Assurance (QA)-approved manner.

20.3.1 All relevant data should be accounted for in the model.

20.3.2 Data may be rejected for the following reasons:

20.3.2.1 Inadequate or unknown quality assurance procedures, and

20.3.2.2 Objective basis, such as statistical analysis for outliers.

20.3.3 Data should be examined for various characteristics before being accepted for inclusion in the model:

20.3.3.1 Where the experimental conditions as planned—did experimental conditions remain within relevant range?

20.3.3.2 Do replicates agree?

20.3.3.3 Are blanks properly accounted for?

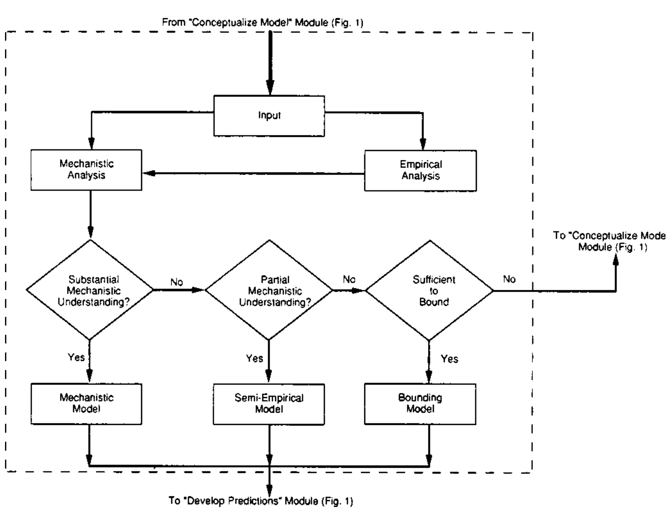

FIG. 3 Details of "Perform Modeling" Module in Fig. 1

20.3.3.4 Is there any evidence of drift testing or analysis?

20.3.3.5 Is the parameter space adequately covered?

20.3.4 Data that cannot be adequately qualified may be used if they are the only data available that address a particular issue, and if the conclusions drawn from them reflect an appropriate degree of uncertainty.

20.4 The results of 20.2 are subjected to mechanistic analysis in conjunction with other data and experience to modify, supplement, or replace the mechanisms initially postulated as responsible for the alterations observed.

20.4.1 The goal is to identify all possible modes of alteration.

20.4.2 For each mode, the following should be identified:

20.4.2.1 Conditions causing the mode to become operational,

20.4.2.2 Parameters that change the rate at which the mode proceeds,

20.4.2.3 Impact of the mode (beneficial, deleterious, innocuous), and

20.4.2.4 Intermodal synergisms.

20.4.3 The model is validated by means of all available data including analog data.

20.4.3.1 Validation of the model means the model can account for all available data. It is preferred that models incorporate substantial mechanistic understanding of the alteration processes.

20.4.3.2 It is likely that, in the initial validation stages, only partial validation will be obtained. The model at this stage would thus be based on partial mechanistic understanding. It is recommended that the process be iterated to improve the model.

20.4.3.3 Upon iteration, it may be found that improvement has been achieved. Iteration should be continued until it is judged that further improvement would have only marginal value.

20.4.3.4 Upon iteration, it may be found that no improvement was achieved.

20.4.3.5 In this practice, with only partial mechanistic understanding, a model is considered to be a semi-empirical model.

20.4.3.6 If the validation and understanding achieved are insufficient, it may be possible to develop models for some other alteration mode and to show that the alteration by this mode is always greater than that for the mode of interest and that there is a preponderance of evidence that this will be true for the time frame of interest. A variation on this approach is to make calculations that permit the conclusion that there is an upper bound to the amount of alteration due to the mode of interest. In either case, the complexity of the modeling a process is decreased for cases in which one or more physical parameters have variable values. For example, in the repository the near-field temperature will eventually decrease as a function of time. If the bounding temperature is chosen as the maximum temperature, then modeling 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, based on a mechanistic interpretation of the process. 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 unstable such that the retarding process is no longer applicable, then this maximum temperature might not yield the bounding degree of alteration and is therefore not a justifiable bounding value. A thorough evaluation of the parameters chosen, and the effect of each parameter on the reaction process, must be documented before the use of the bounding condition.

20.4.3.7 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 (returning to the steps requiring) comparison with short-term data.

NOTE 2—Validation and confirmation of the model should include independent assessment as supported by testing (characterization, accelerated, service condition, or analog, or a combination thereof) and peer review. Independence is defined by the NRC General Technical Position.[10]

20.5 If the model is not suitable for demonstration of self-consistency of data and prediction of long-term behavior (see Section 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

21. Scope

21.1 This element describes the recommended procedure for using the validated model to generate predictions of materials behavior– the predictions required for performance assessment purposes.

21.2 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.

21.2.1 *Model-Testing Predictions*—In the Modeling, Validation, and Confirmation stages of making predictions on behavior, the model is compared with existing experimental data to aid in model development and, ultimately, model validation and confirmation.

21.2.2 *Repository Service Predictions*—After validation, the models will be used to predict the behavior of each material under repository-relevent conditions for license application.

22. The Time Variable

22.1 While, in general, it is likely that test data can be acquired for materials over the expected range of service conditions, it is unlikely that data will extend to long, repository-relevant, times. The degree of extrapolation, in time, for these models is unique. In some cases (for example, corrosion of stainless steels) repository service predictions will have to be made by extrapolation of available data using materials behavior models for which considerable mechanistic understanding of alteration behavior may exist for environments in question.

22.1.1 For materials for which appropriate analogs are available, however, the models are used to interpolate between existing data in order to generate the required materials behavior predictions. 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 (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.

22.2 *Prediction Time*—Since repository system performance requirements (See Section 4 on Summary of Practice) divide the controlled storage time into two periods, one of substantially complete containment and one of the controlled release, the critical period, over which the materials behavior predictions must be made, will depend on the function of the particular material in the engineered barrier system.

22.2.1 For example, the requirement for substantially complete containment may be satisfied mainly by the container materials. Behavior predictions for these materials would therefore be most critical during the containment period, which might be as long as 1000 years (or more) after closure of the repository. However, the behavior of spent fuel and glass play central roles in controlling release and therefore considerably longer term predictions are important for these materials.

22.2.2 Materials behavior predictions will also be required to assess possible interactions between the alteration processes of the various materials in the repository system.

22.2.2.1 For example, it is expected that reactions between the materials of the canister (and container) and the ground water would continue to be important beyond a 1000-year containment period because the resulting perturbation 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.

23.2 Predictions generated from materials behavior models will depend crucially on the particular scenario that is assumed.

23.2.1 For each scenario, the variables that have been identified to affect the particular materials behavior, for example, temperature, groundwater composition, humidity, etc., as functions of time, should be used as input variables for materials behavior models in order to generate predictions.

23.2.2 Materials behavior predictions should be generated for each possible scenario. Methods for combining scenarios are considered to be part of performance assessment and are

[10] Nuclear Regulatory Commission General Technical Position, *NUREG/1297*, "Peer Review for Half–Level Nuclear Waste Repositories."

outside the scope of this practice.

23.2.3 Particular attention should be paid to mutually exclusive repository conditions to avoid unrealistic scenarios.

23.2.3.1 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

24.1 *General*—Every effort should be made to estimate the reliability and level of confidence that can be attached to the materials behavior predictions. This will involve identification of all sources of uncertainty that significantly contribute to the uncertainty in the final predictions and, wherever possible, statistically propagating those source uncertainties through the model to arrive at quantitative estimates of uncertainties in the predictions.

24.2 *Data Uncertainties*—Most data used to develop models will have been taken using tests conducted over comparatively short periods of time, i.e. when compared with the repository time periods. The longer the time over which the test data base is generated, the less will be the uncertainty in parametric values used in behavior models but clearly, as the repository time must greatly exceed test times, this uncertainty can not be decreased significantly unless the alteration mechanisms are clearly understood and incorporated into the predictive models.

24.3 *Parameter Uncertainty*—Parameters are values assigned to independent variables (cf. 9.5) used in a model. Parameters may be based on theory, data, expert judgment or some combination thereof, each of which has its associated uncertainty.

24.3.1 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 *Predictions*—Predictions from models of materials behavior over short periods are expected to be of intrinsically high confidence levels.

24.4.1 Predictions for longer periods of time are expected to have lower confidence levels and will increasingly draw upon the doctrine of reasonable assurance as set forth in the NRC regulations. However, confidence levels will also depend on the particular repository scenario under consideration. 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 *Scenario Uncertainties*—Uncertainties in environment conditions to which materials will be exposed including the dependence of those conditions on time should be evaluated for their contribution to the uncertainty in the final materials behavior predictions.

24.6 *Form of Model*—Uncertainties in the form of the model itself is perhaps the most difficult source of uncertainty to quantify adequately. Emphasis on mechanistic understanding in model development will increase the likelihood that the true form, for the dominant alteration processes, is captured, or at least closely approximated, in the model. However, the confidence with which known or conceivable mechanisms can be excluded for a particular material will determine the uncertainty in the predictions that derive from uncertainties in the form of the model.

24.6.1 There may be potential contributions to alteration from unknown mechanisms which therefore cannot be quantified. However, to the extent possible, the predictions should represent the "state of the art."

CONFIRMATION

25. Scope

25.1 During the pre-closure or operational period for a geologic repository (approximately 70 years) it is expected that additional data will have been accumulated and further advancements in materials science will have been made by the time of confirmation. Such efforts are described in Subpart F, "Performance Confirmation Program," of 10 CFR Part 60 (see 2.3). These data, referred to as confirmation test data in this practice, are intended to provide further confirmation of the model predictions.

25.1.1 Predictions should be revised at that time to reflect possible changes in the materials behavior models arising from the additional data and knowledge.

26. Specific Procedure

26.1 Confirmation test data will be collected while monitoring and testing waste packages as described in 10 CFR part 60.143," Monitoring and Testing Waste Packages."

26.2 A program shall be established at the geologic repository operations area for monitoring the condition of the waste packages.

26.3 Waste packages chosen for the program shall be representative of those to be emplaced in the underground facility.

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

26.5 The WPMP shall include laboratory experiments which 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.

26.6 The WPMP shall also include laboratory experiments which focus on environmental conditions that the waste packages are expected to encounter after permanent closure of the repository.

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

26.8 All confirmation test data shall be compared with the results of predictive calculations based upon models. As necessary the models will be modified so that they can accurately predict all existing long-term data.

26.9 If the comparison is not satisfactory, it will be necessary to return to the Modeling Section of this practice and determine whether the conceptual model can be revised to accommodate the new data.

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 of the U.S. NRC (10 CFR Part 60.151).

27.2 All data collection and predictive modeling shall be done under a qualified Quality Assurance Plan (QAP). The QAP will assure that the quality assurance requirements of the U.S. NRC are met.

27.2.1 ANSI Nuclear Quality Assurance for Waste Management as embodied in RW 0333P, is the preferred standard for a comprehensive quality assurance guide. ASTM standards and other standards can be used in specific instances (for example, laboratory measurements).

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 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 Statements of precision and bias should be developed for quantitative predictions resulting from the application of this practice. (See Practices E 177, E 178, E 583, and DOE/TIC-11400).

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.