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]

[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.

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[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.

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 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

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

[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.

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 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.

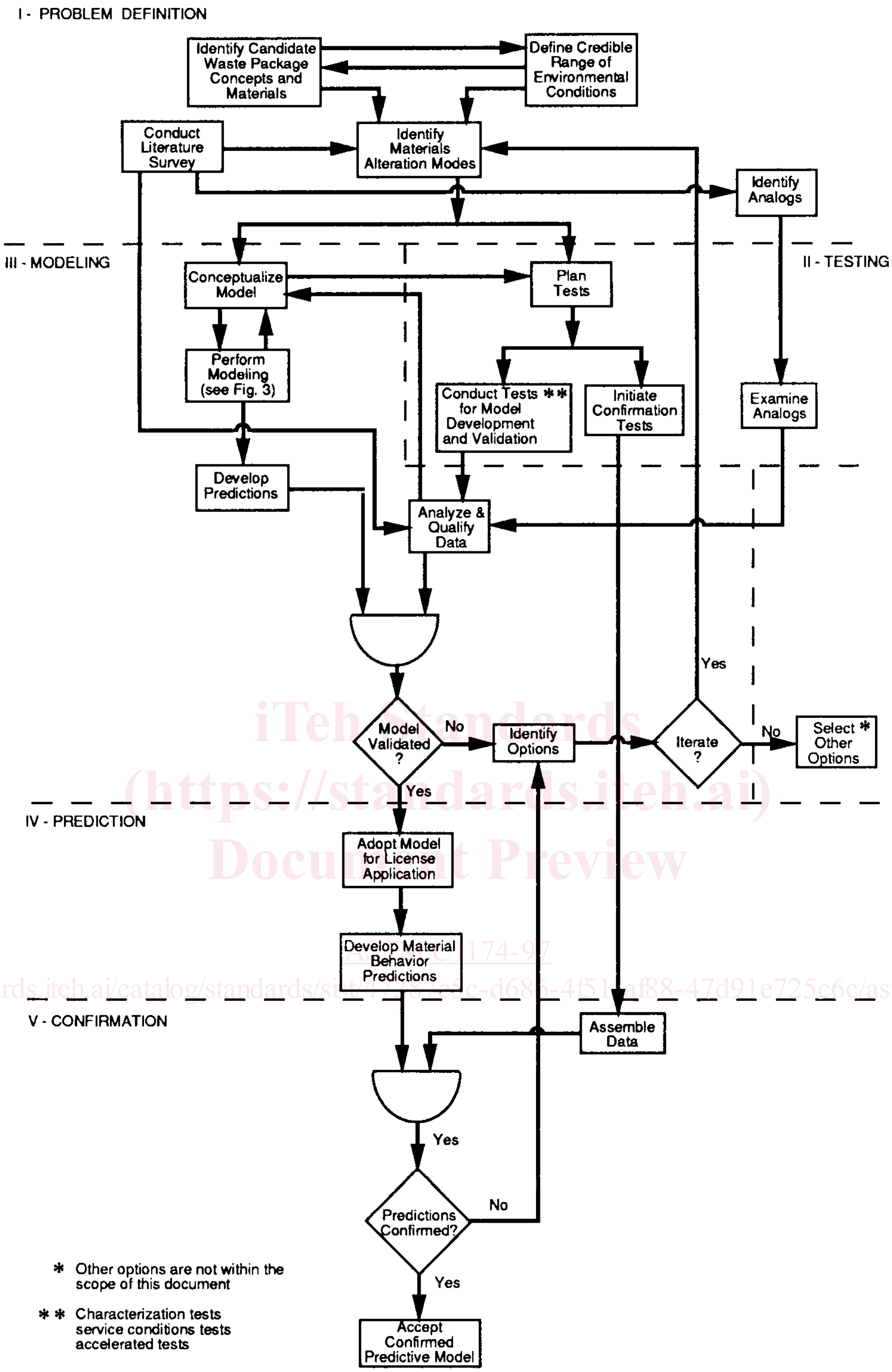

FIG. 1 Logic for the Development of Predictive Models for the Post-Closure Behavior of Waste Package Materials

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 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.