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Standard Guide for Evaluation of Long-Term Behavior of Materials Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste[1]

This standard is issued under the fixed designation C1174; 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 guide addresses how various test methods and data analyses can be used to develop models for the evaluation of the long-term alteration behavior of materials used in an engineered barrier system (EBS) for the disposal of spent nuclear fuel (SNF) and other high-level nuclear waste in a geologic repository. The alteration behavior of waste forms and EBS materials is important because it affects the retention of radionuclides within the disposal system either directly, as in the case of waste forms in which the radionuclides are initially immobilized, or indirectly, as in the case of EBS containment materials that restrict the ingress of groundwater or the egress of radionuclides that are released as the waste forms degrade.

1.2 The purpose of this guide is to provide a scientifically-based strategy for developing models that can be used to estimate material alteration behavior after a repository is permanently closed (that is, in the post-closure period). Because the timescale involved with geological disposal precludes direct validation of predictions, mechanistic understanding of the processes based on detailed data and models and consideration of the range of uncertainty are recommended.

1.3 This guide addresses the scientific bases and uncertainties in material behavior models and the impact on the confidence in the EBS design criteria and repository performance assessments using those models. This includes the identification and use of conservative assumptions to address uncertainty in the long-term performance of materials.

1.3.1 Steps involved in evaluating the performance of waste forms and EBS materials include problem definition, laboratory and field testing, modeling of individual and coupled processes, and model confirmation.

1.3.2 The estimates of waste form and EBS material performance are based on models derived from theoretical considerations, expert judgments, and interpretations of data obtained from tests and analyses of appropriate analogs.

1.3.3 For the purpose of this guide, tests are categorized according to the information they provide and how it is used for model development, support, and use. These tests may include but are not limited to: attribute tests, characterization tests, accelerated tests, service condition tests, and confirmation tests.

1.4 This guide does not address testing required to define or characterize the repository environment (that is, the groundwater quantity or chemistry, host rock properties, etc.). The logical approach and testing concepts described herein can be applied to the disposal system.

1.5 *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, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.6 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

C859 Terminology Relating to Nuclear Materials

C1285 Test Methods for Determining Chemical Durability of Nuclear, Hazardous, and Mixed Waste Glasses and Multiphase Glass Ceramics: The Product Consistency Test (PCT)

C1663 Test Method for Measuring Waste Glass or Glass Ceramic Durability by Vapor Hydration Test

E177 Practice for Use of the Terms Precision and Bias in ASTM Test Methods

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

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

E178 Practice for Dealing With Outlying Observations

E583 Practice for Systematizing the Development of (ASTM) Voluntary Consensus Standards for the Solution of Nuclear and Other Complex Problems (Withdrawn 1996)[3]

2.2 *ANSI Standard:*[4]

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

2.3 *U.S. Government Documents:*[5]

NOTE 1—The U.S. government documents listed in 2.3 and referenced in this guide are only included as examples of local regulations that, depending on the location of the disposal site, may or may not be appropriate. Users of this guide should adhere to the regulatory documents and regulations applicable in the licensing location. The references listed below are explicit examples of local regulations.

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

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

NUREG-1804 Yucca Mountain Review Plan, Rev. 2, NRC ADAMS ML032030389

2.4 *International Documents:*

SKI Report 99:2 Regulatory Perspectives on Model Validation in High-Level Radioactive Waste Programs: A Joint NRC/SKI White Paper, Swedish Nuclear Power Inspectorate, March 1999[6]

IAEA SSR-5 Disposal of Radioactive Waste – Specific Safety Requirements, International Atomic Energy Agency (IAEA), Vienna, Austria, 2011[6]

IAEA GSG-3 The Safety Case and Safety Assessment for the Predisposal Management of Radioactive Waste, International Atomic Energy Agency (IAEA), Vienna, Austria 2013[6]

SSMFS 2008:37 Swedish Radiation Safety Authority Regulatory Code – General Advice, Swedish Radiation Safety Authority, Stockholm, January 30, 2009[7]

Finland Government Decree (736/2008) on the Safety of Disposal of Nuclear Waste, Radiation and Nuclear Safety Authority in Finland (STUK) Helsinki, November 27, 2008[8]

3. Terminology

3.1 *Definitions:*

3.1.1 Definitions used in this guide are as defined in Terminology C859, the *ASTM Online Dictionary of Engineering Science and Technology*[9], or as commonly accepted in dictionaries of the English language, except for those terms defined below for the specific usage of this guide.

3.2 *Regulatory and Other Published Definitions*

3.2.1 Definitions of the particular terms below are generally consistent with the usage of these terms in the context of geological disposal of radioactive materials. If precise regulatory definitions are needed, the user should consult the appropriate governing reference.

3.2.2 *backfill*—the material used to refill excavated portions of a repository after waste has been emplaced.

3.2.3 *buffer*—any substance placed around a waste package in a disposal facility to serve as a barrier to restrict the access of groundwater to the waste package; and to reduce by sorption and precipitation the rate of eventual migration of radionuclides from the waste.

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

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

3.2.6 *engineered barrier system (EBS)*—the man-made, engineered materials placed within a repository (for example, waste forms, waste packages, waste canisters, backfill, buffer materials) that are designed to prevent or inhibit migration of radioactive material from the repository.

3.2.7 *geologic repository—in high-level radioactive waste management*, a system which is used for, or may be used for, the disposal of radioactive wastes in excavated geologic media.

3.2.7.1 *Discussion*—A geologic repository includes the geologic repository operations area, and the portion of the geologic setting that provides isolation of the radioactive waste.

3.2.8 *high-level radioactive waste (HLW)*—generally composed of highly radioactive materials produced as a byproduct of the reactions that occur inside nuclear reactors that are disposed of in a deep geologic repository, such as spent nuclear fuel, and wastes resulting from the reprocessing of spent nuclear fuel.

3.2.9 *risk-informed*—refers to an approach that uses the results and findings of risk or performance assessments to focus attention on those attributes of a geologic repository commensurate with their importance to safety.

[3] The last approved version of this historical standard is referenced on www.astm.org.

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

[5] Available from U.S. Government Printing Office, Superintendent of Documents, 732 N. Capitol St., NW, Washington, DC 20401-0001, http://www.access.gpo.gov.

[6] Available from International Atomic Energy Agency (IAEA), Vienna International Centre, PO Box 100, A-1400 Vienna, Austria, www.iaea.org.

[7] Available from Swedish Radiation Safety Authority (SSMFS), Solna Strandvag 96, 171 16 Stockholm, www.stralsakerhetsmyndigheten.se.

[8] Available from Finlex, www.finlex.fi/en.

[9] Available from ASTM Headquarters, 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428–29593 or www.astm.org.

3.2.10 *scientific investigation*—any research, experiment, test, study, or activity that is performed for the purpose of investigating the material aspects of a geologic repository, including the investigations that support design of the facilities, such as EBS post-closure performance models.

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

3.2.12 *waste form*—the radioactive waste in its physical and chemical form after treatment or conditioning, or both, (resulting in a solid product) prior to packaging.

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

3.3 *Definitions of Terms Specific to This Standard:*

3.3.1 The following definitions are defined only for the usage in this guide, and for the explanation of the analyses contained herein.

3.3.2 *accelerated test*—for the prediction of long-term behavior of materials, a test that results in an increase either in the rate of an alteration process or in the extent of reaction progress when compared with values measured under expected service conditions.

3.3.2.1 *Discussion*—Any changes in the expected alteration mechanism(s) caused by the accelerating test conditions should be accounted for explicitly to clearly justify use of the accelerated test data in model development.

3.3.3 *alteration*—a measurable or visible change in a material affecting its chemical, physical, or radiological properties.

3.3.4 *alteration mechanism*—the series of fundamental chemical or physical processes, or both, by which alteration occurs.

3.3.5 *alteration mode*—for the prediction of long-term behavior of materials, a particular form of alteration, for example localized corrosion.

3.3.6 *analog*—for the prediction of long-term behavior of materials, a material, process, or system that is sufficiently similar to the materials, processes, or systems of interest such that insights gained regarding its condition or behavior can also demonstrate understanding those of the materials, processes, or systems of interest.

3.3.7 *attribute test*—for the prediction of long-term behavior of materials, a test conducted to provide material property data that are required as input to behavior models, but are not themselves responses to the environment, such as density, thermal conductivity, mechanical properties, radionuclide content of waste forms, and so forth.

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

3.3.9 *bounding model*—for the prediction of long-term behavior of materials, 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 being bounded.

3.3.10 *characterization test*—for the prediction of long-term behavior of materials, a test conducted to establish alteration mechanisms for important processes, measure the effects of environmental variables on material changes (alteration) over time, develop process models, and measure model parameter values.

3.3.11 *confirmation test*—for the prediction of long-term behavior of materials, a test for which results are not used in the initial development of a model or the determination of parameter values for a model but are used for comparison with predictions of that model for model validation.

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

3.3.13 *empirical model*—a model representing observations or data from experiments without regard to mechanism or theory. An empirical model may be developed by representing experimental data through regression analysis (that is, using principles of statistics) or to simply bound the observed data.

3.3.14 *extrapolation*—the act of estimating long-term material behavior beyond the range of data collected based on a trend determined by empirical observation.

3.3.15 *in-situ test*—tests conducted within a geological environment representing a potential repository. A special underground laboratory, called an underground research laboratory (URL), may be built for in-situ testing or tests may be carried out in an actual repository excavation. In-situ tests can be used to measure the full range of initial repository environmental properties and material interactions and under natural conditions.

3.3.16 *mechanistic model*—model derived using accepted fundamental laws governing the behavior of matter and energy to represent an alteration process (or processes).

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

3.3.17.1 *process model*—mathematical representation of chemical or physical process that contributes to material alteration.

3.3.17.2 *performance model*—mathematical representation integrating all relevant thermal, chemical, physical, and radiological processes affecting the release and transport of radionuclides from a disposal system.

3.3.18 *model validation*—model calculations and results are compared with independent measurements or analyses of the modelled property to provide confidence that a model adequately represents the alteration behavior of waste package/ EBS materials under particular sets of credible environmental conditions. This provides confidence in the capability of the model to estimate alteration behavior under conditions or durations that have not been tested directly.

3.3.18.1 *Discussion*—Modeling the behavior of an engineered system in a geological disposal facility involves temporal scales and spatial scales for which no comparisons with system level tests are possible: models cannot be 'validated' for times and distances that cannot be observed. 'Model validation' in these circumstances implies showing that there is a basis for confidence in the model(s) by means of detailed scientific bases demonstrating understanding, including external peer reviews, comparisons with appropriate field and laboratory tests, comparisons with observations/tests of analogous materials, conditions and geologies at the process level. Although the term validation has been used in a geological disposal context, the term "validation" has typically been qualified regarding the limitations of its use in the context of geologic disposal. Thus, the term 'validation' is used sparingly in this guide when referring to specific activities that provide support for and confidence in models used for estimating the performance of materials for geologic disposal applications. Section 21 provides further discussion on model validation.

3.3.19 *performance assessment*—systematic evaluation of repository evolution conducted using features, events, and processes (FEP) analyses and performance models to understand better how the performance of individual barriers, components, or attributes of a system impact the overall performance of the system (that is, material behavior models as part of a performance assessment are used to estimate how the engineered disposal system retains/retards radionuclides to limit releases of radionuclides into the environment).

3.3.20 *predict*—estimate the future behavior of a material or released constituent by using a model.

3.3.21 *semi-empirical model*—a model based partially on a mechanistic understanding of an alteration process (or processes) and partially on empirical representations of observations using data from experiments.

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

3.3.23 *service conditions*—environment in which the values of the independent variables are within the range expected during actual service.

4. Summary of Guide

4.1 This guide covers the general approach for proceeding from defining the system to be modelled, through the development, validation, and confirmation of appropriate conceptual process models, to formulation of the material behavior models, and to development of any performance assessment models for the safety analyses. Fig. 1 depicts the various steps in developing a model from defining the system to confirmation of the models during operations and the types of testing that could be used to support model development. This general depiction of model development is used to provide an overall perspective for the contents and discussions presented in this guide and is not intended to be applied in an overly restrictive manner. For example, service condition tests are used to support model formulation. This does not mean that these types of tests cannot also support other steps in model development (for example, providing model support and confidence). Fig. 1 is intended to show how different types of tests are generally used in each step of model development. Some tests may be used to address several modeling needs and serve several purposes. The final step in model development (that is, making long-term estimates of material performance) is also an integral part of a performance confirmation program that is expected to be implemented during the operational period. Such performance confirmation testing includes monitoring the actual materials in the repository environment (for example, waste packages with high-level waste emplaced in the repository drifts). The double arrows in Fig. 1 represent the iterative nature of testing and model development. Although the vertical arrows in Fig. 1 represent the overall progression of model development to its final step of estimating material performance, the entire set of steps can be iterative.

4.2 Fig. 2 provides a more detailed depiction of the iterative nature of model development and categories of tests that are discussed in Sections 7 to 25. Development of the model used to represent material behavior within the overall repository performance model will likely be based on detailed models of the processes that control material degradation in the disposal environment throughout the regulated timeframe. The logical approach described herein can be applied to individual process models, material behavior models, and performance assessment models. The models used for system performance can be conservative or bounding, and potentially simplified from the detailed process models.

5. Significance and Use

5.1 This guide supports the development of material behavior models that can be used to estimate performance of the EBS materials during the post-closure period of a high-level nuclear waste repository for times much longer than can be tested directly. This guide is intended for modeling the degradation behaviors of materials proposed for use in an EBS designed to contain radionuclides over tens of thousands of years and more. There is both national and international recognition of the importance of the use and long-term performance of engineered materials in geologic repository design. Use of the models developed following the approaches described in this guide is intended to address established regulations, such as:

5.1.1 U.S. 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. These barriers include engineered barriers designed to prevent the migration of radionuclides out of the engineered system, and the geologic host medium that provides an additional transport barrier between the engineered system and biosphere. The regulations of the U.S. Nuclear Regulatory Commission for geologic disposal require a performance confirmation program to provide data through tests and analyses, where practicable, that demonstrate engineered systems and components that are designed or assumed to act as barriers after permanent closure are functioning as intended and anticipated.

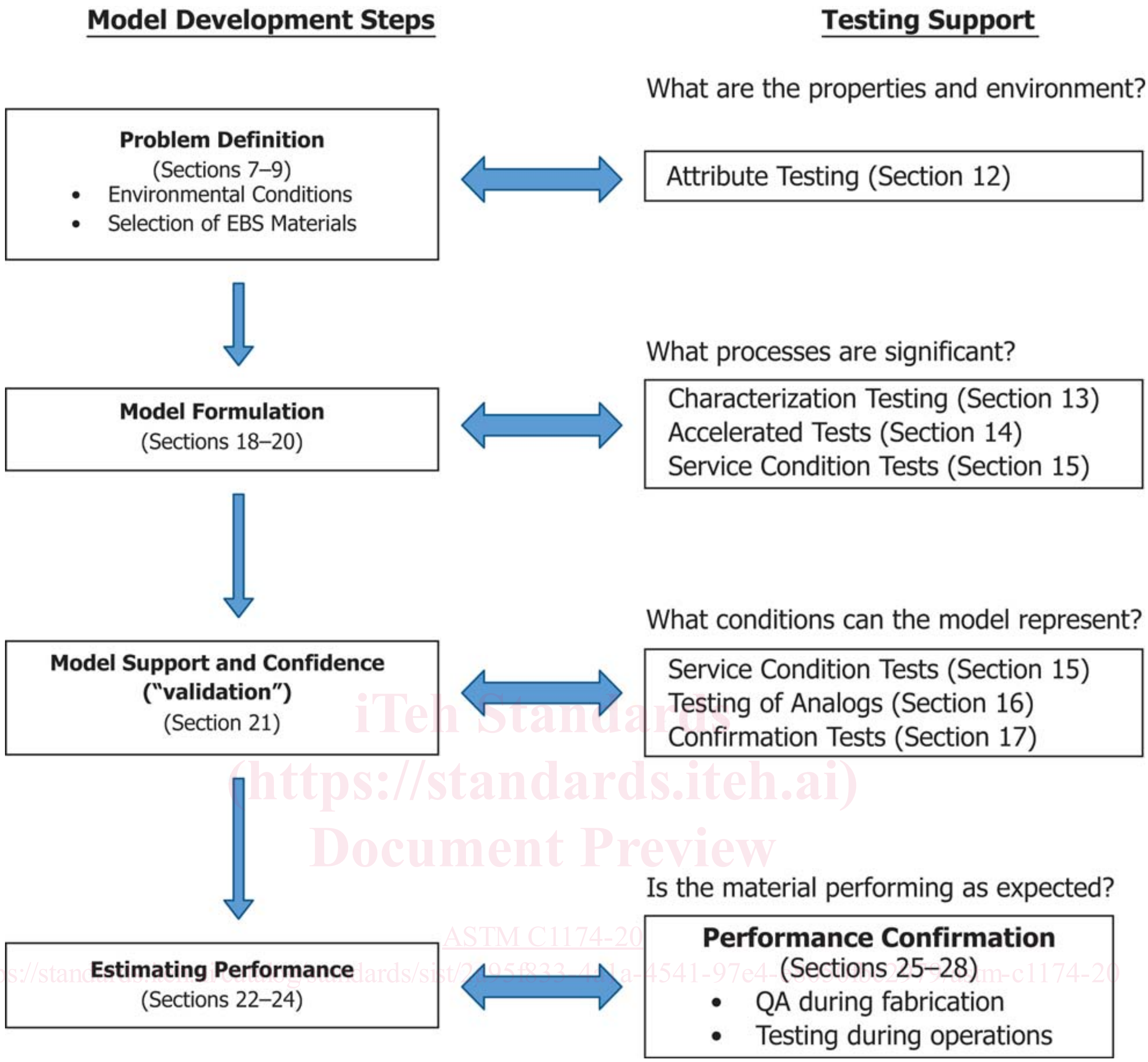

FIG. 1 Model Development Steps and Testing Support

5.1.2 IAEA Safety Requirements specify that engineered barriers shall be designed and the host environment shall be selected to provide containment of the radionuclides associated with the wastes.

5.1.3 The Swedish Regulatory Authority has provided general advice to the repository developer that the application of best available technique be followed in connection with disposal, which means that the siting, design, construction, and operation of the repository and appurtenant system components should be carried out so as to prevent, limit, and delay releases from both engineered and geological barriers as far as is reasonably possible.

5.1.4 The Regulatory Authority in Finland identified the need to support the safety assessment stating that the input data and models utilized in the safety case shall be based on high-quality research data and expert judgement. Data and models shall be validated as far as possible and correspond to the conditions likely to prevail at the disposal site during the assessment period.

5.1.5 The Office of Nuclear Regulation in the United Kingdom will regulate an operating geological repository under the Nuclear Installations Act through application of the Safety Assessment Principles developed for all nuclear facilities and the post-closure disposal period will be regulated under the Radioactive Substances Act by the Environmental Agency. A Memorandum of Understanding outlines how the two regulators work together[10].

5.2 This guide aids in defining acceptable methods for making useful estimations of long-term behavior of materials from such sources as test data, scientific theory, and analogs.

[10] Office for Nuclear Regulation, onr.org.uk.

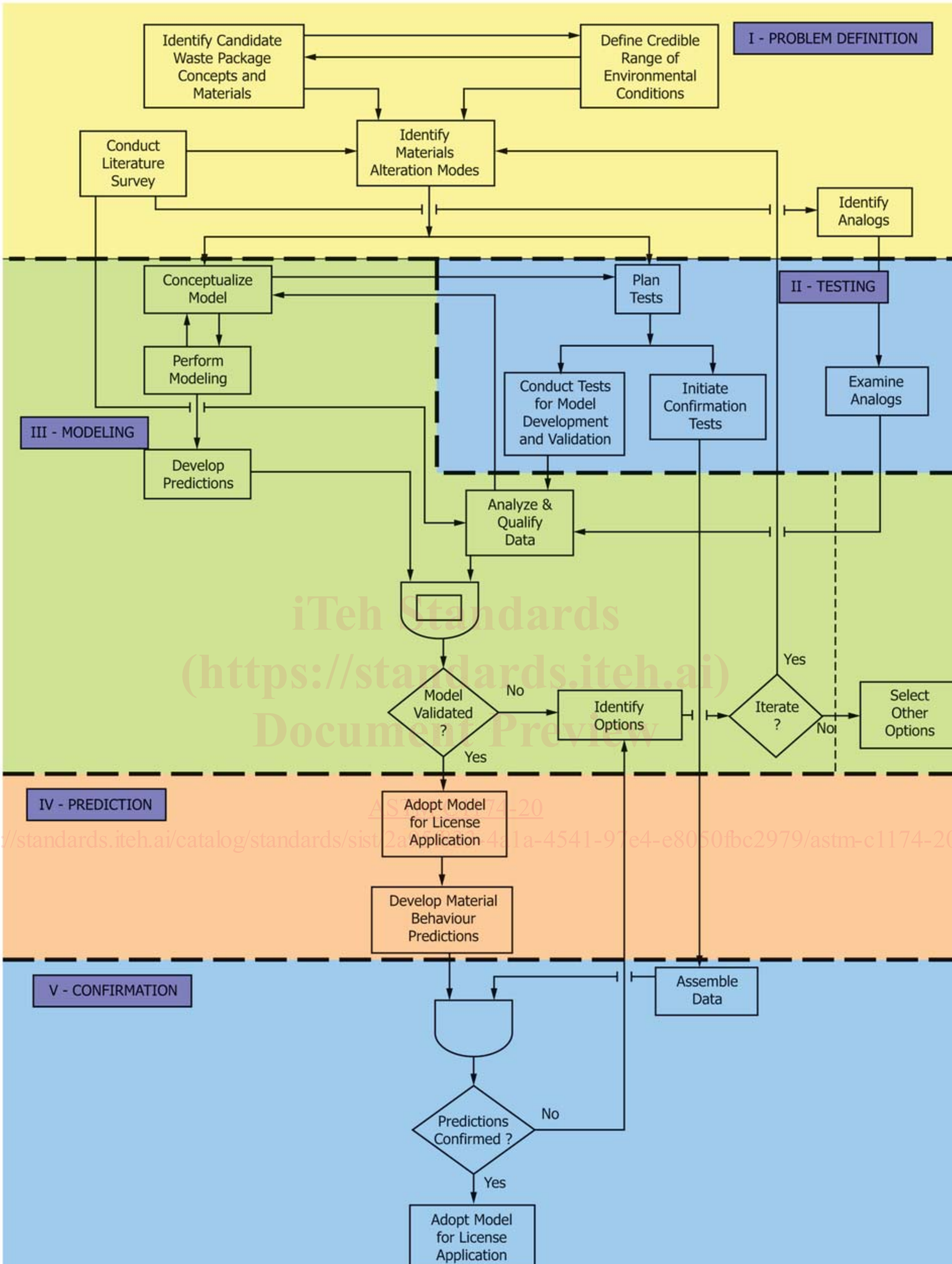

FIG. 2 Logic for Development of Models for Estimating Alteration Behavior of Materials

5.3 This guide recognizes that technical information and test data regarding the actual behavior of EBS materials will by necessity be based on test durations that are short relative to the time periods required for geologic disposal (for example, thousands of years and longer). In addition to use in formulating acceptable long-term performance models, data from short-term tests are used to support EBS design and the selection of materials. For example, low confidence in the ability to model the degradation of one material may justify the selection of alternative EBS barrier materials that can be modelled with higher confidence. It is expected that the model will correctly represent material behavior in the intended applications of establishing design criteria, comparison of performance assessment results with safety limits, and so forth. See Section 21 for further discussion on model support and confidence.

5.4 The EBS environment of interest is that defined by the natural conditions (for example, minerals, moisture, biota, and mechanical stresses); changes that occur over time, during repository construction and operation, and as a consequence of radionuclide decay, namely, radiation, radiation-induced damage, heating, and radiolytic effects on the solution chemistry; and changes that may occur over the post-closure period. Environmental conditions associated with disruptive events (for example, mechanical stress from seismic events) and processes (for example, changes in water chemistry) should also be considered.

6. General Procedure

6.1 This guide outlines a logical approach for estimating the behavior of materials over times that greatly exceed the time over which direct experimental data can be obtained. It emphasizes the use of models that are based on an appropriate mechanistic understanding of the processes involved in long-term alterations of materials used under repository conditions. That often requires the use of accelerated tests conducted under more aggressive conditions than expected to occur in the repository.

6.2 The major elements in the approach to develop models for estimating the long-term behavior of EBS materials are problem definition, testing, modeling, performance estimate, and confirmation. Fig. 2 is a flow chart showing the logical approach for model development followed in this guide. Although it is not expected that the structure of Fig. 2 will apply exactly to every situation, especially as to the starting point and the number and type of iterations necessary to obtain acceptable alteration models, it is likely that the development of models for most materials will include these major elements. Details on the individual elements are given in Sections 7 to 26. Development of performance models will likely be conducted under a quality assurance program as discussed in Section 27. The total uncertainty of a performance model includes conceptual uncertainties (that is, those related to how well the form of the model represents the process(es) controlling material degradation), parameter uncertainties (for example, those in the data used to determine model parameter values), and uncertainty in initial/boundary conditions (for example, the environmental service conditions to which the model is applied). The consequences of these uncertainties with regard to the performance of the disposal system are used to determine the uncertainty in the risk. These are discussed in Section 24.

PROBLEM DEFINITION

7. Scope

7.1 The objective of the problem definition is to identify the materials and environments to be assessed and the system to be modeled.

7.1.1 An extensive list of features, events, and processes (FEPs) that should be considered for inclusion in the system model has been compiled and is being utilized world-wide. Many of these FEPs are generic (that is, not specific to a particular site or material), but provide a reasonable starting point for developing system-specific FEPs that address the materials and site conditions being investigated.

7.2 In this guide, methods are recommended for the development of models to evaluate the long-term alteration of EBS materials proposed for use in the geologic disposal of high-level radioactive wastes. This guide describes a methodology for constraining the performance of materials proposed for use in systems designed to contain or control the release of radionuclides.

7.3 Problem definition includes identifying factors that define the system to be modelled to support evaluations of longterm behavior of repository materials during the post-closure period. This can be done using literature surveys and other sources of information helpful in characterizing the alteration of EBS materials. The key steps include the following:

7.3.1 Identify potential environmental conditions (including the natural system conditions and any EBS materials effects on those) to which the material may be exposed. The alteration behavior of a material will depend on the environment in which it is used. The environment within a disposal system will be affected by naturally occurring conditions and events and by the alteration of EBS components. For example, the chemistry of groundwater that contacts the waste forms will be significantly affected by reactions with the natural materials, thermal effects of waste emplacement, corrosion of EBS materials, and radiolysis. The anticipated range of repository environments throughout the post-closure period should be defined and the model developed using test conditions that evaluate degradation behavior within this range to the extent practical. That range of anticipated environments is referred to herein as the service conditions. Additional tests under conditions outside the service conditions should be considered to further determine the functional dependencies of processes represented in the models on environmental variables.

7.3.2 Identify possible EBS design concepts.

7.3.3 Identify EBS Barrier and other materials. The various materials to be evaluated for use in the systems, structures, components, and barriers that are designed and deployed to contain radionuclides within the repository environment must be identified. A risk-informed approach to repository performance assessment can be used to identify the behavior characteristics of those materials that may substantially impact risk-based performance measures by affecting the release of radionuclides from the repository during the post-closure period. Performance assessments can analyze the sensitivity to specific materials and alteration processes and disruptive events (for example, seismic activity) to identify those attributes of particular EBS materials that are most important for limiting the release of radionuclides over the long time periods of geologic disposal. The subject of this guide is evaluating those aspects of the long-term behavior of these materials that most significantly impact the risk-based performance measures.

7.3.4 Identify the inventory, composition, and condition of the waste forms.

7.3.5 Identify dominant material alteration modes. Modeling the alteration behaviors of EBS materials having degradation characteristics that are determined to be important to waste isolation needs to be performed with sufficient accuracy and precision to determine the useful lifetimes and expected performance of these materials. All relevant degradation processes need to be understood sufficiently so that the impact of these materials is not under-estimated and modeling outputs can be used to provide reliable input to risk-based decision making / optimization. The alteration behaviors of EBS materials having degradation characteristics that are determined to be unimportant to waste isolation do not need to be modelled with the same accuracy and precision as those materials deemed to be important to waste isolation.

7.3.6 Identify behavior of appropriate natural analog materials.

8. General Considerations

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

8.1.1 *Environment*—The geologic environment should be evaluated by characterization of the initial environment and mechanical condition with consideration of the effects of time and alteration of EBS and waste form materials on the environment. Use of ranges in the values of such environmental conditions as temperature, groundwater chemistry, microbiology, and colloid content may be needed to account for changes in the environmental conditions that occur over time naturally due to degradation of EBS components and disruptive events (for example, seismic activity). A special underground laboratory, called an underground research laboratory (URL), may be built to enhance characterization activities and for in-situ testing or tests to be carried out in a representative repository excavation.

8.2 *Conceptual Designs*—A general concept for an initial EBS design expected to meet regulatory requirements can be developed based on current understanding of the conditions of a particular site and the performance of EBS materials under those conditions.

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

8.3.1 Insights from natural analogs might be available to provide early guidance regarding the long-term alteration of EBS materials in the repository environment.

8.3.2 The selection of materials for the EBS could be influenced by known degradation behaviors. This approach could lessen the need for hard-to-achieve high confidence levels in material performance. For example, a container material that exhibits a moderate but predictable general corrosion rate under anticipated disposal conditions might be selected for use as a corrosion barrier because the thickness of the wall could be engineered to provide containment for an acceptable time.

8.4 *Ranges of Materials Property Values and Environmental Conditions*—Frequently, a range of parameter values will be needed to characterize material behavior under environmental conditions that could occur during disposal.

8.4.1 *Ranges*—A range of parameter values may be used to represent uncertainties in environmental conditions or material properties. For example, environmental conditions may include anticipated temporal and spatial variability and the waste form properties may be described using ranges that take into account variations in composition.

8.4.2 *Bounding Conditions*—Bounding conditions represent the anticipated extreme credible values of material and environmental parameters or variables. These furnish necessary input for estimating performance limits. However, thorough evaluations of all important material attributes and their effects on the anticipated alteration mechanism are required to ensure that the calculations representing bounding conditions do indeed provide performance limits. For example, the extreme low value of the range of environmental pH values considered (for example, pH 3) does not correspond to the pH value that gives the lower limit of the glass dissolution rate (for example, pH 7). Additionally, it is important to ensure that the combinations of boundary conditions/parameter values that are considered avoid non-physical or contradictory conditions that could lead to unrealistic model results, such as large volumes of water being present at temperatures exceeding the local boiling point.

8.5 *Available Data*—A substantial amount of data related to both the materials of interest, including the waste forms, and the extant environmental conditions may be available (for example, in the technical literature) before the initiation of tests for model development. Insight gained from evaluating available data can be used to design characterization and accelerated tests for use in the development of the model for long-term performance.

8.5.1 *Interactions*—The process of predicting materials behavior in repositories must involve consideration of interactions between materials and environments. For example, interactions between various materials and the environment may lead to the formation of reaction products that affect the environment. Interactions between different materials within the EBS may be direct, in the case of materials that are in physical contact, or indirect through the groundwater chemistry. That is, changes in the groundwater due to corrosion of one material will affect the corrosion behavior of other materials that the groundwater contacts. Characterization tests should be conducted to ensure that the range of environmental parameters represents the impacts of relevant processes, events, and EBS material corrosion.

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

8.7 *Preliminary Models*—For each important alteration process, preliminary models shall be developed to represent and evaluate steps in the process, postulates, and inferences related to either observed or expected behavior of the materials in the proposed environments. Preliminary models could use conservative approaches that would be used to help focus further model development and data collection in those areas that are most important to safety. More realistic models (that is, less conservative) could evolve as model development and data collection proceeds. More realistic analyses would provide insight into the conditions that may occur and insights into the safety margins of bounding assessments.

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

9. Specific Procedure—Problem Definition (See Fig. 2)

9.1 *Define Credible Range of Environmental Conditions*—Determine the range of environmental conditions to which the material will be exposed during the operational (pre-closure) period (that is, as relevant to the initial state of, and initial conditions for, the post-closure Engineered Barrier System) and after permanent closure (that is, the post-closure period). The range should include initial environmental conditions and changes that will occur over time due to changes in climate, radiolysis of air and groundwater, corrosion of EBS components, and so forth. The extent of such interactions may be difficult to quantify initially, but should be noted and accounted for in a final model.

9.1.1 Features, Events, and Processes (FEPs) relevant to degradation and alteration of the EBS components should be identified. The FEPs can be used to identify the environmental variables to be considered (for example, temperature, chemical constituents, and mechanical loads) and to help identify the degradation processes to be evaluated and relevant test conditions.

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, activities to address performance issues pertinent to each option can be incorporated into subsequent modeling and testing steps to inform future decisions. For example, the values of some parameters will differ depending upon whether waste package emplacement geometry is vertical or horizontal.

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

9.4 *Identify Possible Alteration Modes*—Use technical literature to help identify possible alteration modes for the materials of interest relevant to the environmental conditions for the repository site being evaluated.

9.5 *Identify Variables*—Identify the variables regarded to be important to material behavior in the disposal system, for example, the amount of water expected to contact a waste glass. For each independent variable, identify the expected range of values.

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

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

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

TESTING

10. Scope

10.1 *Model Confidence*—The confidence in model results will depend upon both how well the model represents the alteration mechanism under the in-service conditions (for example, type or stoichiometry of corrosion product, form of alteration layers, mode of degradation), how well the dependencies on environmental variables are represented in the model, and how well the values of environmental variables used in the model represent the in-service environmental conditions (for example, temperature, groundwater chemistry, groundwater quantity).

10.1.1 The ability of the behavior model to provide reliable estimates will be strongly dependent on the accuracy with which the mathematical form of the model represents the process rates (for example, the degree to which the model is based on a mechanistic understanding of the alteration process), the accuracy with which test methods quantify the process rates, uncertainties in the test data used to derive the parameters and parameter values used in the model, and the uncertainties in how accurately tests represent the actual in-service conditions for which the model is applied (see Section 24 on Uncertainties).

10.1.2 Testing of EBS materials is required to establish the effectiveness of these materials to retain radionuclides within the repository environment or limit their releases, or both. Tests conducted over a comparatively short period, for example, less than 20 years, will be used to support development of performance models for materials behavior in the repository environment. To the extent possible, those models are based on a mechanistic understanding of material durability and tests designed to quantify long-term performance based on that understanding. Test results are not extrapolated to longer times. Rather, they are used to parameterize models that represent the kinetics of processes that control material degradation. The testing program must address the development, scientific basis, and confirmation of these models.

10.1.3 Materials testing programs should be designed with the goal of supporting the validation and verification of materials behavior models, as well as minimizing uncertainties in the test data, the models, and the use of the models in calculations of long-term behavior in the repository environment.

10.2 *Types of Tests*—Testing of EBS materials (Fig. 1) will be required for a variety of reasons and is expected to include a variety of tests referred to herein as: attribute tests (Section 12), characterization tests (Section 13), accelerated tests (Section 14), service condition tests (Section 15), testing of analogs (Section 16), and confirmation tests (Section 17).

11. Reserved

12. Attribute Tests

12.1 *General*—Estimation of the response of materials to the repository environment during the post-closure period will require the specification of the intrinsic properties ("attributes") of the materials. These properties are not expected to change over time in response to the repository environment.

12.1.1 Examples of material attributes are density, thermal conductivity, chemical composition, radionuclide content, and all mechanical properties.

12.1.2 Attribute tests are designed to provide specific information on attributes of test materials necessary for the development of the behavior models when reliable data are not available from the literature. It is expected that most of the required information concerning barrier materials (for example, steels), spent fuel, and high-level waste material attributes will be available in the literature, but measurements of some properties may be required.

12.2 *Specific Procedure-Attribute Tests:*

12.2.1 Identify the material properties required to apply the model.

12.2.2 Examine the literature for materials properties and evaluate which property values may be used unambiguously without further testing.

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

12.2.4 Compile the values for all properties that may be required as input to modeling.

13. Characterization Tests

13.1 *General*—Characterization tests have the primary function of providing a mechanistic understanding of the important processes of material alteration expected in the repository environment, developing analytical models to represent those processes, determining model dependencies on environmental variables and material attributes (such as composition), and measuring parameter values for the anticipated range of service conditions. These tests are used to establish the basic mathematical form representing the process in the behavior model.

13.1.1 *Purpose*—Characterization tests are designed to identify EBS alteration mechanisms that could occur in a repository and the dependence of those processes on environmental conditions and material attributes.

13.1.2 Characterization tests are used to determine the processes/mechanisms controlling long-term alteration under expected repository conditions, support the selection and parameterization of an appropriate analytical model, quantify dependencies on material properties and environmental variables, and assess the uncertainties.

13.1.3 The ranges of test conditions shall exceed the expected range of repository conditions to investigate the sensitivity of the alteration mechanisms to variations in the values of particular test parameters and add confidence to the modeled dependencies.

13.2 *Specific Procedure-Characterization Tests:*

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

13.2.2 Perform tests to identify alteration processes/mechanisms that occur in the repository environment conditions.