Designation: C1174 – 17

Standard Practice for Evaluation of the 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 practice 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 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 practice 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, the post-closure period) because the timescales involved with geological disposal preclude direct validation of predictions.

1.3 This practice also addresses uncertainties in materials behavior models and the impact on the confidence in the EBS design criteria, the scientific bases of alteration models, 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 practice, 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: accelerated tests, attribute tests, characterization tests, confirmation tests, and service condition tests.

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

1.5 *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)

C1682 Guide for Characterization of Spent Nuclear Fuel in Support of Interim Storage, Transportation and Geologic Repository Disposal

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

E178 Practice for Dealing With Outlying Observations

E583 Practice for Systematizing the Development of

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

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

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

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*[9]—Definitions used in this practice are as currently existing in Terminology C859, or as commonly accepted in dictionaries of the English language, except for those terms defined below for the specific usage of this practice.

3.2 *Regulatory and Other Published Definitions*—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.

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

3.2.2 *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.

3.2.3 *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.

3.2.4 *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.

3.2.5 *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.

3.2.6 *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.

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

3.2.7 *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.

3.2.8 *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.

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

3.2.10 *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.

3.2.11 *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.

3.2.12 *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 practice, 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 expected service conditions.

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

3.3.3 *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 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, general corrosion, localized corrosion.

3.3.6 *analog*—for the prediction of long-term behavior of materials, a material, process, or system whose composition and environmental history are sufficiently similar to those anticipated for the materials, processes, or systems of interest to permit use of insight gained regarding its condition or behavior to be applied to the material, process, or system 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, and develop 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 or may be developed to bound all the observed data.

3.3.14 *extrapolation*—the act of estimating long-term material behavior beyond the range of data collected based on 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.

3.3.18 *model validation*—the process through which 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*—Modelling 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 that which 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 external reviews and comparisons with appropriate field and laboratory tests, and comparisons with observations of tests and 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 practice and when used is referring to the activities taken to 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 (support for and confidence in models).

3.3.19 *predict*—estimate the future behavior of a material by using a model.

3.3.20 *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.

3.3.21 *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.

3.3.22 *service condition tests*—for the prediction of long-term behavior of materials, a test conducted to determine what material properties and alteration processes are likely to be important under environmental conditions expected during the performance period.

4. Summary of Practice

4.1 This practice covers the general approach for proceeding from the statement of a problem in estimating the long-term behavior of materials, through the development, support, and confirmation of appropriate models, to formulation of the material performance models. Fig. 1 depicts the various steps in developing a model through 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 and testing is used to provide an overall perspective for the contents and discussion presented in this practice and is not intended to be applied in an overly restrictive

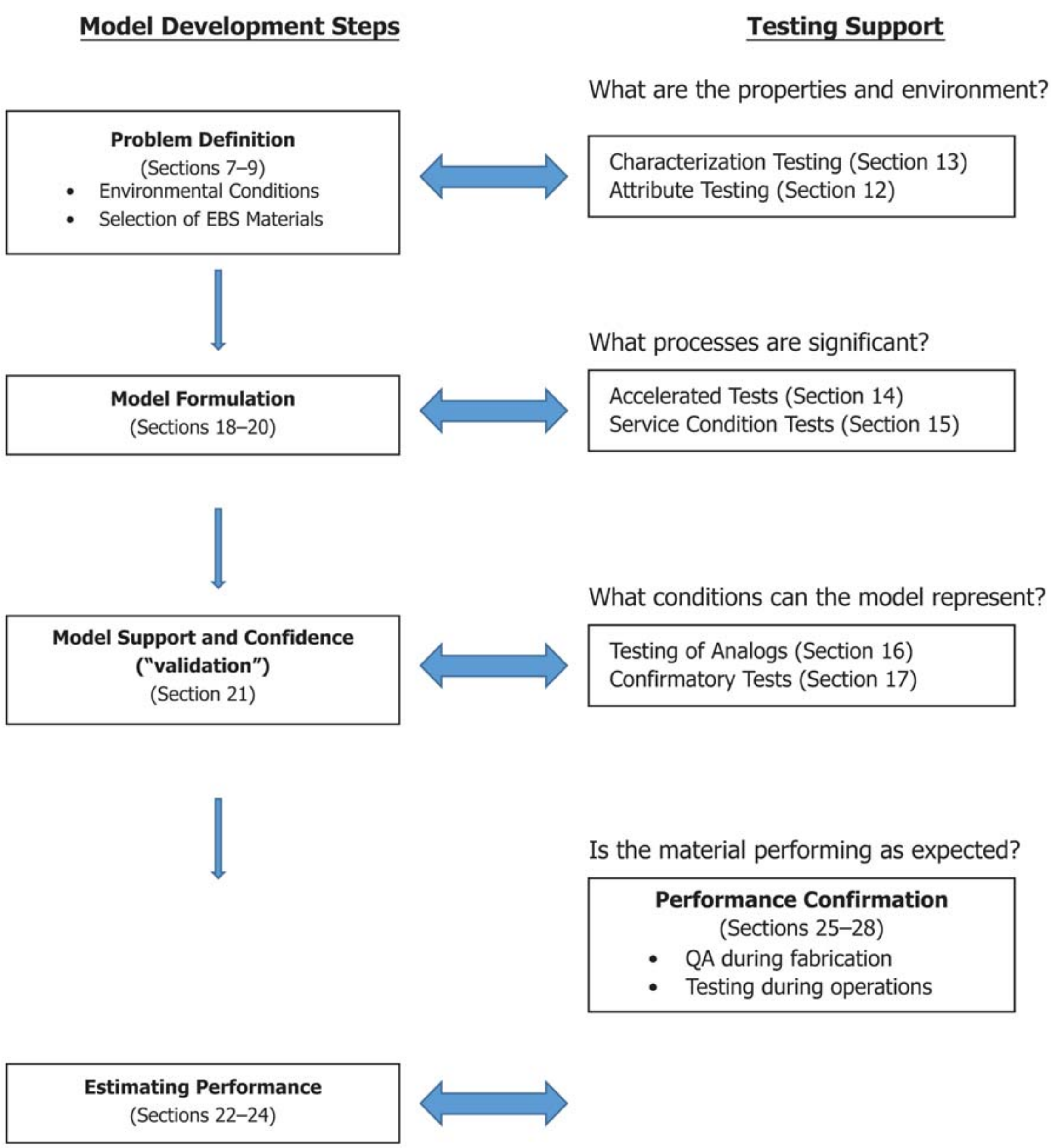

FIG. 1 Model Development Steps and Testing Support

manner. For example, certain tests (for example, service conditions tests) are depicted as supporting model formulation; however, this should not be interpreted that these types of test would also not be able to provide support for other steps in model development (for example, model support and confidence). The figure is intended to correlate the types of tests and steps of model development in a general sense. Clearly, some tests may assist multiple modeling needs and purposes. The final step in model development (that is, long-term estimates of material performance) is correlated to a performance confirmation program that is expected to be implemented during the operational period and, at least in part, allow for monitoring of 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 are used to represent the iterative nature of testing and model development. Although the steps in model development process can also be iterative, the vertical arrows in Fig. 1 are used to represent the progress of model development to its final step (estimating performance of the materials). Fig. 2 provides a more detailed depiction of the iterative nature and model development and testing.

5. Significance and Use

5.1 This practice 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 practice 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 practice 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.

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. The two regulators have a Memorandum of Understanding outlining how the regulators work together (onr.org.uk/wastemanage/position-statement.pdf).

5.2 This practice 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.

5.3 This practice 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 the EBS design and selection of materials. For example, low confidence in a degradation model for one material may justify the selection of alternative EBS barrier materials that can be modelled with higher confidence. It is expected that the data and model will reflect the intended application of establishing design criteria, comparison of performance assessment results with safety limits, etc. 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 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 practice.

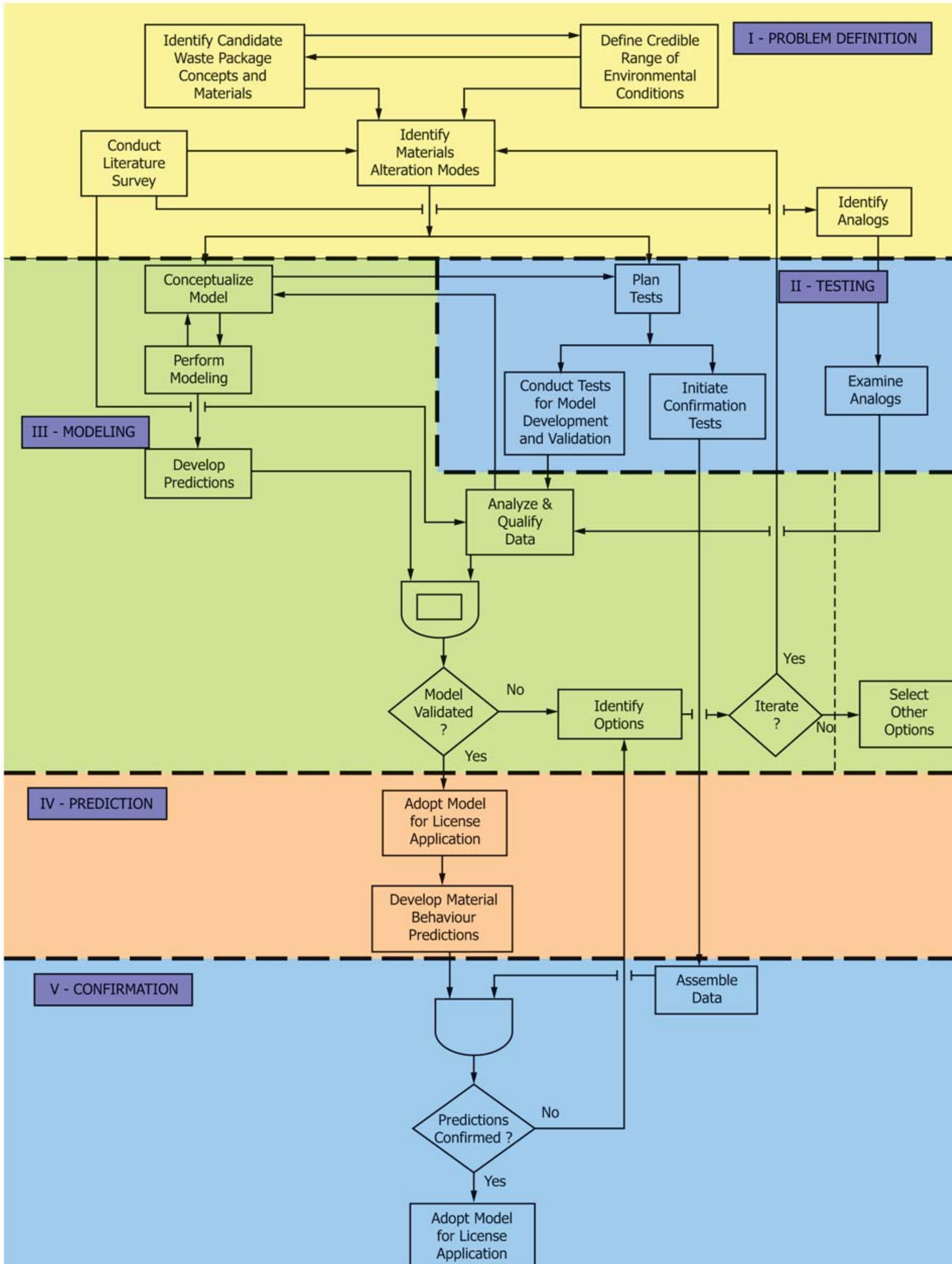

FIG. 2 Logic for the Development of Models for Estimating the Alteration Behavior of Materials

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 contain these major elements. Details on the individual elements are given in Sections 7 – 26.

Development of performance models will likely be conducted under a quality assurance program as discussed in Section 27. An important aspect of performance models is the uncertainty of the model, including uncertainties in the form of the model, the data used to determine model parameters, and 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.

6.2 *Identification of Materials:*

6.2.1 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 contribute to risk by affecting the release of radionuclides from the repository over 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 the attributes of particular EBS materials that are most important for limiting the release of radionuclides over the long time periods of geologic disposal. It is the long-term behavior of these risk-significant materials that is the subject of this procedure.

6.2.2 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 underestimated 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.

6.3 *Identification of Credible Ranges for Environmental Conditions:*

6.3.1 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 both the natural conditions and events, the design and materials used in the EBS, 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, the 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 results representing this range to the extent practical.

PROBLEM DEFINITION

7. Scope

7.1 The objective of the problem definition is to identify the materials and environments to be assessed and the processes, interactions, and alteration modes that should be included in the models. This information is used to design conceptual models and design tests to develop and evaluate process models. An extensive list of features, events, and processes (FEPs) that should be considered has been compiled and utilized world-wide; however, many of these FEPs lists tend to be more generic than specific to a particular site or material. A generic FEPs list is a reasonable starting point for developing more site and material specific FEPs that would be expected to address the specific materials and site conditions being investigated.

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

7.3 Problem definition includes identifying factors that are important in the development of models to support evaluations of long-term 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 factors include the following:

7.3.1 Identification of potential environmental conditions to which the material may be exposed,

7.3.2 Identification of possible EBS design concepts,

7.3.3 Identification of EBS materials,

7.3.4 The identity, composition, and condition of the waste forms,

7.3.5 Identification of potential materials alteration modes, and

7.3.6 Identification of appropriate natural analog materials.

7.4 This practice 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 accelerated tests and the use of models that are based on an appropriate mechanistic understanding of the processes involved in long-term alterations of materials used under repository conditions.

8. General Considerations

8.1 *Site Characterization*—A potential repository site must be investigated with respect to its geologic, hydrologic, seismic, etc. conditions that could affect the performance of the repository. For purposes of this practice, 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 shall be evaluated by characterization of the initial environment and mechanical condition and consideration of the effects of time and alteration of EBS and waste form materials on the environment. Ranges in the values of such environmental conditions as temperature, groundwater chemistry, microbiology, colloid content, and disruptive events (for example, seismic activity) may be needed to account for changes in the environmental conditions that occur over time. 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 EBS design can be initially developed to meet regulatory requirements based on current understanding of: (*1*) the conditions of a particular site, and (*2*) the performance of EBS materials under the site 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. Since these materials serve the function of containment and control of potential radionuclide release rates, their alteration behavior under the set of conditions expected in the repository over long time periods must be reliably determined and the alteration modes understood. This understanding is developed by first reviewing both the available information regarding the environmental conditions and the effects of the environment on the candidate materials.

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

8.3.2 The selection of materials for the EBS could be influenced by the support and confidence for degradation rate models. This approach could lessen the need for hard-to-achieve high confidence levels in a degradation model. For example, a container material that exhibits a moderate but predictable rate of general corrosion, but is not susceptible to localized corrosion, might be selected for use as a corrosion barrier and the thickness of the wall engineered to provide for a 'corrosion allowance.'

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

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

8.4.2 *Bounding Conditions*—Bounding conditions represent the anticipated extreme credible values of a range of parameter or variable values. These furnish necessary input for estimating performance limits. However, thorough evaluations of the alteration mechanisms, all important material attributes, and the effects of these attributes on the anticipated alteration processes are required to ensure that the calculations representing bounding conditions do indeed provide performance limits. For example, the pH value that gives the lower limit of the glass dissolution rate (for example, pH 7) may not be the extreme value of the range of environmental pH values considered (for example, pH 3). Additionally, it is important to ensure that the combination 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 *Preliminary Testing*—A substantial amount of data related to both the materials of interest, including the waste forms, and the extant environmental conditions may be available before the initiation of tests for model development. Various preliminary modeling and testing efforts can be conducted to understand specific aspects of the material/environment system and make preliminary evaluations of the alteration processes. Insight gained from the preliminary tests and evaluations 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, in turn, become part of the environment. Interactions between different materials within the EBS may be direct, in the case of materials that are in physical contact, or indirect through the groundwater chemistry. That is, changes in the groundwater due to corrosion of one material will affect the corrosion behavior of other materials that the groundwater contacts. Of course, it is possible that thermal or mechanical effects on EBS materials could be more important than corrosion processes, which could increase the significance of seismic events. Characterization tests should be conducted to ensure that the range of environmental parameters represents the impacts of relevant processes and events.

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. 1)

9.1 *Define Credible Range of Environmental Conditions*—Determine the range of environmental conditions to which the material will be exposed during (*1*) the operational period, as appropriate, and (*2*) 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, etc. 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 determine the range of environmental conditions (for example, temperature, chemical constituents, and mechanical loads) 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 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 components. 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 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.

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 kinetics (for example, the degree to which the model is based on a mechanistic understanding of the alteration process), uncertainties in the test data used to derive the parameters and parameter values used in the model, and the uncertainties in representations of 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 contain radionuclides in 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. 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 This practice does not address testing required to define (or model) the repository design or environment (that is, the groundwater quantity or chemistry, host rock properties, etc.). The testing concepts described herein do not specifically address the testing of integrated systems within the EBS. It is expected that the logical approach in this practice can be applied to integrated systems.

10.3 *Types of Tests*—Testing of EBS materials will be required for a variety of reasons and thus are expected to include a variety of tests, such as: attribute tests, characterization tests, confirmation tests, and service condition tests.

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, mechanical properties, etc.

12.1.2 Attribute tests are designed to provide specific information on 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 properties may be unambiguously determined without 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 and measuring model dependencies and parameter values. These tests are used to establish both the suitability and 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.

13.1.2 Test conditions may differ significantly from the expected repository conditions, and so it may be necessary to investigate the sensitivity of the alteration mechanisms to variations in the values of particular test parameters. Extending test parameter ranges could also be useful for: (*1*) evaluating cliff-edge effects just outside the expected parameter ranges, and (*2*) demonstrating continuity of mechanisms over the ranges used in accelerated tests.

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 mechanisms that occur in the repository environment conditions.

13.2.3 Analyze the quantitative and qualitative information from the characterization tests and identify the alteration mechanism(s) occurring under the test conditions.

13.2.4 Identify material and environmental variables affecting the alteration rate. Conduct tests using ranges of values to determine the kinetic dependencies.

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

14. Accelerated Tests

14.1 *General*—The purpose of an accelerated test is to increase the rate of one or more alteration process or the reaction progress without changing the mechanism(s) of the alteration process under investigation. Therefore, some knowledge of the mechanism that is operative under in-service conditions is needed for the design of the accelerated test and meaningful use of accelerated test data. Processes may be accelerated by changing various test parameters relative to their in-service values, including temperature, material surface area, mechanical loads, solution volume or flow rate, initial solute concentrations, humidity, etc. Care should be taken to ensure, to the extent practical, that the test method and test conditions do not alter the mechanism of the process that is being accelerated (for example, characterization tests, as discussed in Section 13, may be useful in identifying potential limitations in accelerated tests).

14.1.1 If the alteration mechanism that is operative in the accelerated test differs from that which is operative under the in-service conditions or changes over a range of accelerating test conditions, the accelerating test conditions and response must be evaluated to determine if and how the change is related to the process being accelerated. In many cases, changes in the process can be detected using trends in the response as the accelerating test parameter is varied.

14.1.1.1 Temperatures higher than the expected service conditions are often used to accelerate the rate of corrosion of a material. The effect of increasing the test temperature can be represented using an Arrhenius plot to detect changes in the effective activation energy, which may indicate a change in mechanism.

14.1.1.2 Other test results indicate changes in mechanism that may or may not impact the process being evaluated. Consider a series of accelerated tests conducted at different temperatures in which dissolution of a primary phase resulted in formation of corrosion product *A* at repository-relevant conditions but in formation of corrosion product *B* at temperatures above a critical temperature T°. If the process being accelerated is affected differently by formation of corrosion products *A* and *B*, for example, by the release of the soluble species j into solution, the accelerated tests in which *B* forms are not applicable. If which product phase forms is irrelevant to the dissolution rate of the primary phase, the accelerated tests above T° may be applicable.

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

(1) Alter the state of a material in a short time to simulate exposure to repository conditions over long time periods, and thereby produce artificially "aged" materials. (This may be desirable for determining the 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, such as after a large seismic event.),

(2) Measure the rates of slow reactions within reasonable laboratory time-scales,

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

(4) Promote the approach to solution saturation, and

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

14.1.2.1 An example is the exposure of samples of spent fuel to conditions that accelerate alteration relative to repository conditions (such as high temperature, high solution Eh, crushing to expose grain boundaries and increase surface area, etc.) to obtain upper limit values for radionuclide release upon exposure to groundwater. The effects of each accelerating condition on the dissolution rate should be quantified and mechanistically described.

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

14.1.4 *Models*—Results of accelerated tests can be used to develop or support a performance model by demonstrating conditions under which materials perform well or perform poorly. They can also be used to demonstrate when an alteration process can be excluded from the model or provide bounding parameter values.

14.1.4.1 As an example of excluding a process, a test for stress corrosion cracking (SCC) of a candidate waste container material might establish that the initiation of SCC can only occur under temperatures that are higher and aqueous chemistries that are more aggressive than those that can plausibly occur in the repository.

14.1.4.2 An example of alteration model parameter measurement might be a test for general corrosion that is conducted at a higher level of anodic polarization than expected to occur in the repository. From the data, best-fit values could be obtained for making a determination of an bounding corrosion current density using a mathematical model for general corrosion that incorporates passivation and passivation breakdown processes. This would provide support for and confidence in using the model for long-term assessments.

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

14.2 *A Specific Procedure for Accelerated Testing:*

14.2.1 Define possible alteration mechanisms.

14.2.2 Identify the alteration process to be accelerated, method to accelerate, parameters that can be used for acceleration, and alteration indicators (for example, extent of corrosion based on weight change).

14.2.3 Identify the type of test(s) and range of test conditions to be used in the accelerated test (for example, select conditions to isolate the effects of an individual variable).

14.2.4 Perform tests using a set of parameter values expected to increase rate of process relative to service conditions.

14.2.4.1 Compare the nature and extents of alteration attained within the series of tests conducted using the range of accelerating parameter values and, if relevant, with alteration attained in tests using parameter values that represent service-conditions.

14.2.4.2 Verify that the variations in process evaluated using the accelerated tests is relevant and can be related to the mechanisms expected to be operative under service conditions.

14.2.5 Identify the range of test conditions to which the accelerated behavior applies and compare with the postulations in 14.2.2.

14.2.5.1 Show that the process is relevant to the mechanisms expected to occur under disposal conditions, taking into account anticipated changes in the environment to which the materials of interest will be exposed.

14.2.5.2 If the alteration mechanisms observed in the accelerated tests differ from those assumed in the process model, reevaluate the relevance of the process model, the test method, and the test conditions used to accelerate the process to the service conditions and return to 14.2.2 to iterate on this procedure until a satisfactory accelerated test method is developed.

14.2.6 Provide results as input to the modelling activity.

15. Service Condition Tests

15.1 *General*—The purposes of service condition testing are to determine variables that affect corrosion behavior, identify those that must be represented in the alteration model (either explicitly or implicitly by using lumped variables), and establish a database for determining the alteration mechanism operative under repository-relevant conditions. These may include laboratory tests under conditions simulating disposal conditions, lysimeter tests, tests in underground research laboratories, burial tests, etc.

15.1.1 These tests are used to identify the key aspects of the materials and the environment that affect the alteration mechanisms under expected conditions. Observations of the alteration mechanisms under service conditions can be used to determine the relevance of accelerated tests results (and the mechanisms observed therein) for developing alteration models and deriving alteration model parameter values.

15.1.2 Service condition tests should be designed to measure the dependence of material behavior on as many potentially relevant environmental conditions as practical to identify important environmental variables.

15.1.3 Service condition tests establish the values of key environmental variables to be used as the reference case for long-term confirmation testing (see Section 13).

15.1.4 Service condition tests may provide data for alteration of materials under actual repository test conditions with which models can be confirmed, for example, short-term *in-situ* tests conducted in underground research laboratories.

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

15.2 *Specific Procedures-Service Condition Tests:*

15.2.1 Select test conditions. "Normal" test conditions may be defined in terms of ranges that include maximum, average, and minimum values anticipated for each key variable.

15.2.1.1 Conduct sufficient number of tests to measure responses spanning the full range of normal conditions for each variable.

15.2.1.2 Compile and evaluate the data obtained for understanding of the materials alteration behaviors. Results obtained in tests conducted under normal environmental conditions may be used as reference values for tests conducted under conditions outside the normal range to accelerate alteration, understand the alteration mechanism, or evaluate the dependence on key variables.

16. Analysis and Testing of Analogs

16.1 *General*—When estimates of long-term performance are made based on models obtained using the results of characterization, accelerated, and service condition tests, confidence in the performance estimates over many thousands of years could be considerably enhanced through the analyses of natural and man-made analogs. For analog materials to be useful, reliable information should be available concerning their age, chemical composition, and exposure history. The material properties can be determined by using attribute testing as described in Section 10, but determination of exposure conditions, such as solution compositions, contact time, and temperature, is outside the scope of this practice.

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 that is over 100 years old, iron objects exist, including enriched in nickel, that may have some applicability to selected alteration behaviors.

16.1.2 The analyses of analogs can be useful in determining whether different mechanisms can control alteration 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 test responses of analogs can provide confidence in an experimental method for accelerating corrosion behavior and in the models used for particular alteration modes.

16.1.3.1 A good use of analogs would be to provide additional confidence in the sensitivity of model results to a range of material and environmental conditions. It is unlikely that analogs will be found that are identical in composition and conditions of exposure to the EBS materials in the repository. For example, natural uranium minerals might be used as analogs for the alteration of uranium dioxide spent fuel, but such an analysis should recognize that such minerals did not evolve in a geochemical environment that included close proximity to zirconium metal. The sensitivity of test responses of natural uranium minerals in the presence and absence of zirconium would indicate their usefulness as analogs.

16.1.4 Characterization of the short-term behavior of analog materials in laboratory experiments could be used to establish that the analogs behave similarly in natural and experimental environments. This would support the conclusion that the relevant mechanisms have been taken into account in the model. However, any conclusions must give due consideration to survivor bias as well as the representativeness of the exposure conditions of the analog to the material under study.

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

16.2.1 *Identify Analogs*—Identify natural or man-made analogs appropriate for the material and alteration mode under investigation.

16.2.1.1 Search existing literature for potential analogs. Include work in other disciplines, such as archaeo-metallurgy, geology, and history.

16.2.1.2 Analyze the degree of similarity and evaluate 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 applicable and available.

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

16.2.3.1 Dating of site,

16.2.3.2 Geology of site and depth of burial,

16.2.3.3 Sample storage conditions following retrieval, and

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

16.2.4 Characterize the analogs, including:

16.2.4.1 Photographic documentation of specimens and of retrieval process,

16.2.4.2 Dating of specimens and time of exposure,

16.2.4.3 History of specimens and environmental exposure, including nature of water contacting material, contact time, temperature, etc.,

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

16.2.4.5 Bulk chemical composition analysis of analog,

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

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

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

16.2.6 Analyze the data, for example:

16.2.6.1 Estimate the rate of alteration of the analogs,

16.2.6.2 Determine the mechanism(s) of alteration, 16.2.6.3 Compare the data from tests of analogs with data from tests of the candidate materials or waste forms, and

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

17. Confirmation Tests

17.1 *General*—Confirmation tests are designed to produce materials alteration data to support application of the alteration model to the EBS system after the initial formulation and use of the model developed for demonstrating compliance repository safety during the post-closure period. Testing (particularly *in-situ* testing) should be continued as long as practical and necessary during the pre-closure period of the repository but prior to permanent closure of the repository, to confirm key aspects of the behavior of the EBS materials used in models for estimating the EBS performance during the post-closure period. Also, tests that had begun as service condition tests could be extended to serve the purpose of confirming the estimated materials alteration behavior.

17.1.1 *Use*—Confirmation tests, which are to be conducted prior to permanent closure of the repository, are used to provide data showing the alteration model is appropriate for representing material behavior during the post-closure period.

17.1.1.1 They would generally be conducted *in-situ* (such as, within an exploratory shaft facility at the repository site) or under the full suite of conditions expected to be present within the repository. Confirmation testing provides further support for the integrated alteration behavior of materials independent of the data collected to support license application analyses.

17.2 *Specific Procedure-Confirmation Tests:*

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

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

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

17.2.4 Examine material alteration and compare with the behavioral model results (see Performance Confirmation Section 25). 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 analyses of long-term behavior model(s).

MODELING

18. Scope

18.1 Modeling may be performed on a risk-informed basis to estimate the effects of alteration processes on systems, structures, and components that contribute to waste isolation. Modeling may also be performed in support of EBS designs.

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

18.2.1 It is expected that development of models and generation of test data will be an iterative process. Preliminary models could use conservative approaches that would be used to help focus further model development and data collection on those aspects determined to have the greatest impact on safety. More realistic models (generally less conservative) could evolve as model development and data collection proceeds.

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

19. General

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

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

19.2.1 Characterization test data,
19.2.2 Accelerated test data,
19.2.3 Service condition test data,
19.2.4 Analog test data,
19.2.5 Confirmation test data, and
19.2.6 Literature information.

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

19.3.1 *Mechanistic Models*—In purely mechanistic models, the dependent variables are related to independent variables through individual or coupled processes that have been identified, are understood, and have scientific bases. The relationships are expressed using mathematical representations for chemical or physical processes. A purely mechanistic model for a process can be represented mathematically by Eq 1:

$$Y = F(x_1 \ldots x_n), \quad (1)$$

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

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

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

19.3.2.1 A semi-empirical model uses mechanistically-based terms for some processes, while other processes are represented by terms based on empirical observations. Semi-empirical models represent a practical compromise between mechanistic and empirical models. These models are illustrated mathematically by Eq 2:

$$Y = f(x_i \ldots x_n) + \varepsilon, \tag{2}$$

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

19.3.2.2 The approach for developing a semi-empirical model is to postulate a series of steps or reactions as being representative of the processes expected to have the greatest impact on long-term behavior. Relationships between the dependent and independent variables having the form of Eq 2 can be inferred by scientific reasoning that describes those steps. This is done by conducting characterization tests to measure the effects of important variables and determine the forms of the functions $f(x_i)$ that minimizes the residual term.

19.3.3 *Empirical Models*—Purely empirical models describe the observed material responses and dependencies on variables without reference to a mechanism. Purely empirical models appear frequently in the technical literature to quantify trends in material behavior. These models often serve as a first step towards the development of a mechanistic model to represent the observed trend. An empirical model can have the same mathematical form as mechanistic and semi-empirical models; the difference is the functional dependencies on the variables (denoted as g) are not based on theory or a mechanistic model, Eq 3:

$$Y = g(x_i \ldots x_n) + \varepsilon \tag{3}$$

The residual term ε represents the difference between the response calculated by using the mathematical expression and the measured response Y. The coefficients are determined by optimizing the responses in characterization tests conducted using values of the variables that span their ranges in the service condition to minimize the residual. The mathematical form of an empirical relationship between the measured responses and variable values may provide insight into mechanisms that may control the alteration. For example, the observation of a dependence on the square root of test duration may be indicative of control by a diffusion process with constant diffusivity.

19.3.3.1 The approach for empirical models is to determine a relationship that is consistent with or provides an upper bound to observed data within an acceptable margin. A model is considered to be purely empirical when a mechanistic relationship between the variables and response cannot be postulated or inferred. The correlation between the variable and the response is analyzed empirically to determine a possible functional relationship. The independent variables that affect a particular response may initially be chosen on the basis of judgment, inconclusive data, or some partially applicable theories. Other variables may become apparent during testing. For example, it might be hypothesized that the corrosion rate of a certain steel should be affected by temperature, pH, chloride [Cl^-] concentration, and Eh of the water to which it is exposed. A possible conceptual model could have the following mathematical form, Eq 4:

$$dY/dt = \mathrm{F\,B(Eh)\,A(T)\,P(pH,\,Cl^-)} + \varepsilon \tag{4}$$

where dY/dt is the corrosion rate (for example, mil/y), B(Eh) is a function relating the measured corrosion current to the solution Eh, F represents the constants in Faraday's Law, A(T) is the temperature dependence, and P(pH, Cl^-) is a function relating the catalyzing and inhibiting effects of pH and Cl^- (for example, on the formation of a passive layer), and ε represents the residual between the measured rate and the model due to approximations and processes not taken into account.

19.3.3.2 The functional forms determined in empirical models may only be applicable under the test conditions used to generate the data. That is, the values of unidentified variables that are taken into account by the residual may be different under different test conditions. In the example in 19.3.3.1, the rate may depend on the chromium content of the steel. The composition of the steel may be taken into account in the value of B, P, or ε in the rate expression depending on how the electrochemical and chemical processes are affected.

19.3.3.3 Consider the case where the steel corrosion rate depends on the solution Eh according to the Butler-Volmer model. In that case, the Eh-dependence in the empirical function B(Eh) can be represented using the Butler-Volmer equation, which also accounts for the temperature dependence of the oxidation reaction. Replacing the B(Eh) term with the Butler-Volmer equation will affect the A(T) term and probably also the P and ε terms. Additional characterization tests may be required to determine lumped parameter values for different representations.

20. Development of a Materials Behavior Model

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

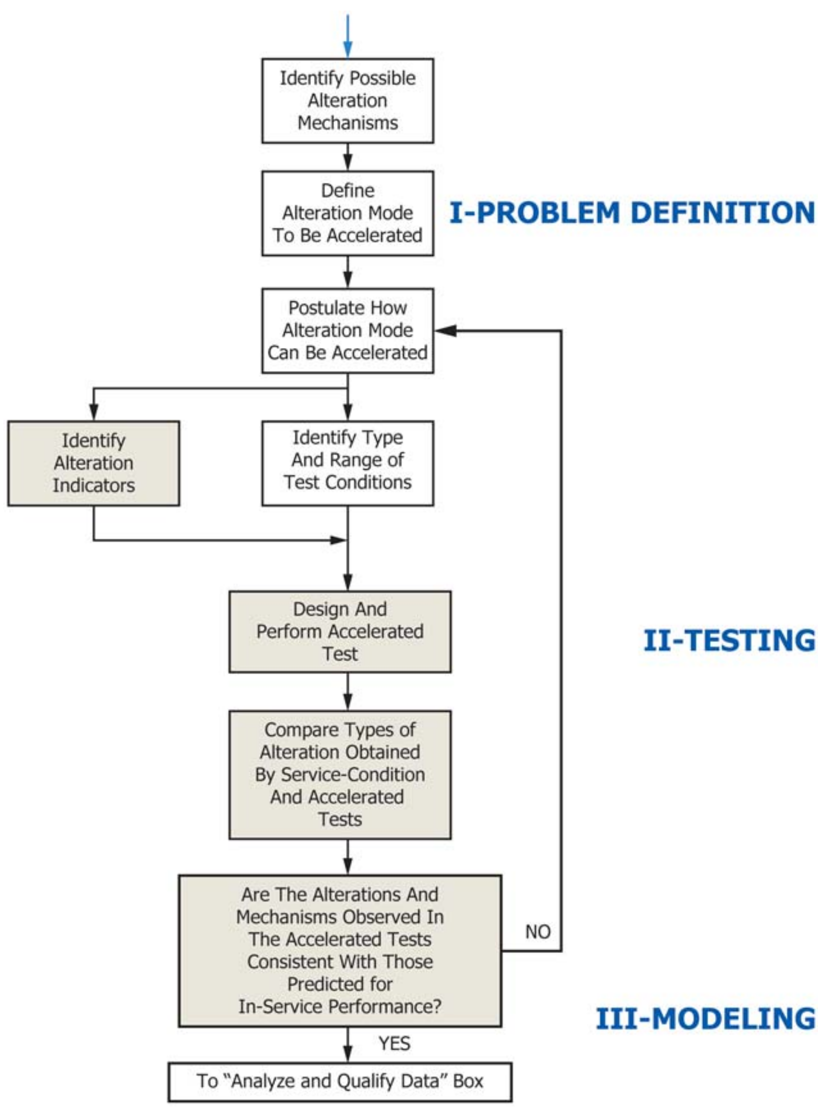

FIG. 3 Recommended Procedure for Developing Accelerated Tests for Materials

process in more detail. Depending on the level of mechanistic understanding of the alteration processes, a model may be considered empirical, semi-empirical, or mechanistic.

20.1.1 Empirical analysis of the conceptual model is usually the initial step taken because the significant variables are generally unknown or uncertain. In this case, the data from service condition and characterization tests, and possibly from other sources (for example, attribute tests and natural analogs) are analyzed to identify relationships and trends in the data. The consistency between the expected behavior from the conceptual model and the observed trends in the data is used to evaluate the adequacy of the model and provide insights to modify the model as necessary.

20.1.2 Another objective of empirical analysis is to look for evidence of changes in the relationship between the independent variables and the test response as the values of test variables (for example, temperature and pH) are changed. This may indicate a change in the alteration mechanism and is particularly important for the analysis of accelerated test results. Identification of trends in the data during empirical analyses may lead to hypotheses of mechanistic relationships. The conceptual model may be modified to take these relationship into account and other experiments designed to test the hypotheses. The empirical conceptual model may thereby evolve into a semi-empirical model.

20.2 All data used to develop the final process models and determine model parameter values important to waste isolation should be collected in a Quality Assurance (QA)-approved manner (see Section 27). Preliminary tests and analyses used to develop initial conceptual models do not need to be qualified.

20.3 Data may be rejected on the basis of inadequate test controls or on an objective basis, such as statistical analysis to identify outliers. Data that are not fully qualified may be used if they are the only data available that address a particular issue, are adequate for their intended use in formulating the model, and conclusions drawn from them are assigned an appropriate degree of uncertainty. Data not originally developed under the required QA program may potentially be qualified for use in model and parameter development and validation as allowed by procedures of the implementing organization.

20.4 Confidence in the empirical model can be provided using analyses methods such as Expert Elicitation.[10]

21. Model Validation (Support for and Confidence in Models)

21.1 Model validation is the process in which model results are compared with independent measurements or analyses. Validation provides support for and confidence in the application of the model to acceptably estimate the alteration behavior for conditions that cannot be tested directly. In supporting the

[10] Kotra, J. L., Lee, M. P., Eisenberg, N. A., and DeWispelare, A. R., "Branch Technical Position on the Use of Expert Elicitation the High-level Radioactive Waste Program, NUREG-1563, US NRC, Washington, D.C., 1996.

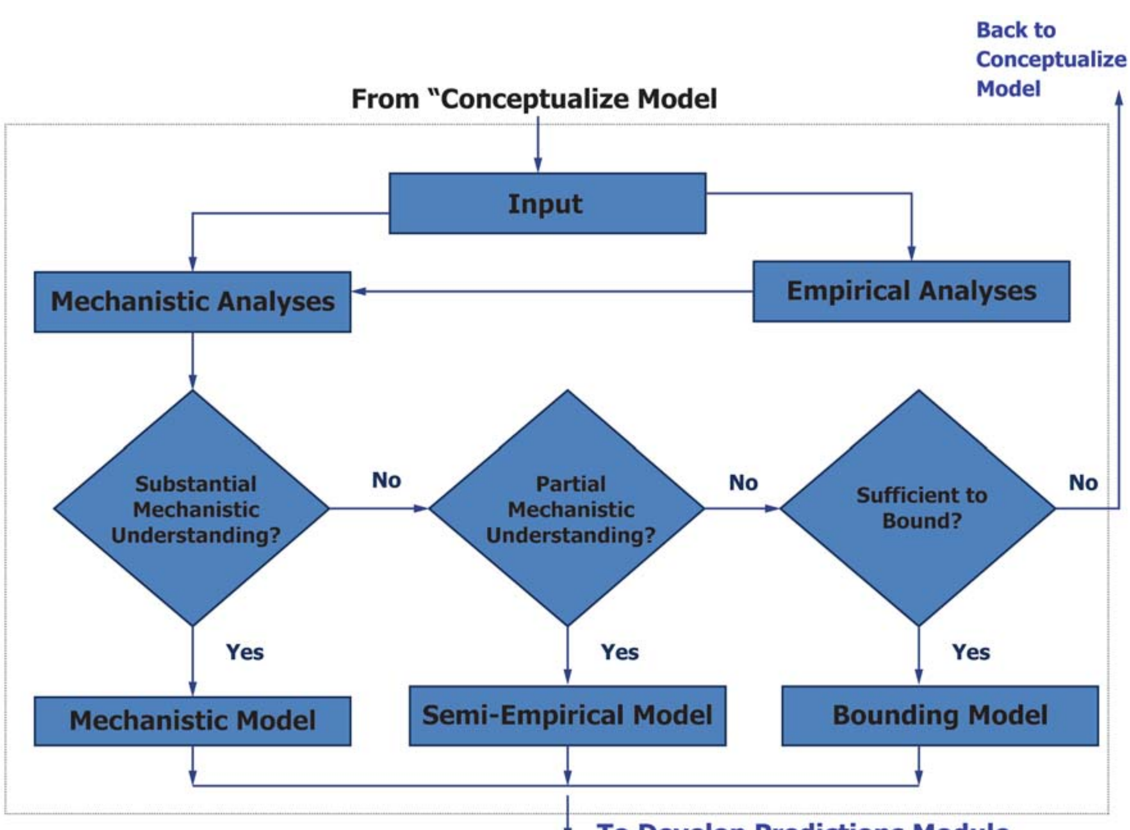

FIG. 4 Details of "Perform Modeling" Module in Fig. 1

material alteration models developed using the techniques described above, it should be recognized that "validation" (or proof in the traditional sense) in terms of comparison of model result with a material response measured over the full range of expected in-service conditions is obviously impossible when one of the key conditions is the post-closure time period of thousands of years. Instead, support for and confidence in model results is based on comparisons of the results of in-service condition, *in-situ*, and confirmation tests and analysis of analogs—making allowance for the long time periods and modeling uncertainties—is the general standard that the models should be required to meet. Thus, the term 'validation' is used sparingly in this practice and when used is referring to those activities that provide support for and confidence in models used for estimating the performance of materials for geologic disposal applications.

21.1.1 Support for and confidence in models is enhanced when multiple lines of evidence are provided (for example, laboratory test, in situ tests, analog tests).

21.2 The models are generally derived using data limited to tests conducted for durations that are very short compared to the very long times to which the models will be applied. Many material behavior properties do not depend on time directly. Instead, they depend on environmental conditions that may change over time in the disposal system within expected ranges (for example, temperature, mechanical loads, and pH). Although the values of environmental variables will vary within expected ranges over time, the dependence of the material response on those variables will not change unless the mechanism changes. Confidence in models for these processes can be enhanced by conducting tests under conditions that span the full range of environmental conditions anticipated to occur over the long service life of the disposal system. Confidence in the predictive capacity is usually higher for mechanistic models than for empirical models because of the relationships between the variables and the test response can be attributed to specific processes. However, the same test data can often be interpreted using different models that predict different long-term behavior. For example, although the dissolution rates of borosilicate glasses are known to depend on temperature, pH, and the activity of dissolved silica, there is an on-going debate whether the dissolution rate is controlled by surface dissolution reactions or diffusion through surface layers. Dissolution rates measured over the full range of temperatures, pH values, and silica concentrations (up to saturation concentrations) are represented equally well with the two mechanisms. Furthermore, changes in the mechanism may occur as alteration progresses that cannot be predicted by a mechanistic model, such as the nucleation of a secondary phase that affects the glass dissolution rate. In this case, the model providing the higher upper bound may be preferred to provide the more conservative analyses.

21.3 Support for and confidence in some materials behavior models may be obtained using natural analogs. For example, an alteration model for the degradation of commercial spent fuel might be based on test data in which mineral phases formed as a result of the dissolution of uranium dioxide generating saturated solutions. The composition of these phases can then be compared to the known compositions of U-bearing mineral phases known to occur in the repository environment to support the aspect of the model representing the effects of alteration phases. However, confidence in the model based on analog information will typically have some inherent limitations that must be acknowledged when documenting the model support. For example, the analog information described here is limited because the naturally-occurring uranium phases did not evolve in close proximity with other materials that will be present in the EBS, such as zirconium cladding and stainless steel containment materials.

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

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

21.5 Support for and confidence in material behavior models may also be provided by the use of accelerated tests. For example, a waste container material could be exposed to water or water vapor at a temperature higher than the anticipated in-service condition. The corrosion product resulting from the test could then be compared to that estimated by the model for in-service conditions, and, if similar, could be used to provide support for and confidence in the corrosion model as providing an upper bound for the long-term repository conditions.

21.6 It should be recognized that all models are essentially simplified representations of actual alteration processes. Models developed under the foregoing procedures may be superseded by models that better represent the process or are more efficiently implemented. Should a new model give results that conflict with the results obtained from the initial model, the new model must be supported by comparing model results with the same test data used to validate the previous model. Additional tests may be required to discriminate between alternative models.

21.7 If no representation model can be developed that is consistent with the test data, it may be necessary to return to the Problem Definition stage (see Section 9). The appropriateness of the test data should be re-evaluated. 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. The Swedish and United States regulatory authorities (SKI and NRC) have provided regulatory perspectives on model validation in the high-level radioactive waste management programs.

ESTIMATING PERFORMANCE

22. Scope

22.1 This element describes the recommended procedure for using models to estimate materials behavior for performance assessment purposes. Generally, there will be two broad categories of models used in estimating performance of materials behavior. A first category of model are 'process-type' models used to represent individual EBS materials under in-service conditions in a detailed manner to support the identification of important processes and parameters affecting their alteration. These models are based on testing during development and confirmation activities. Although these models could be used directly in performance assessments, these process-type models tend to be more detailed than is required in performance assessments that represent the overall repository system. A second category of models are those that are further simplified (based on the identified important processes and parameters) for use in performance assessment models because they are more efficient for use in probabilistic evaluations of overall performance. These 'performance assessment' models are used to represent the alteration behaviors of the EBS materials having the greatest impact on system performance, as identified via the 'process-type' models. Model development is an iterative process and it can be expected that understanding and information learned with either the process models or the performance assessment models can be used to assist development and support for both models. However, this SP is applicable more to the process-type model that represents a smaller subset of the overall performance model and generally has a limited set of processes that can be evaluated in material testing.

22.1.1 The process models can be used to compare measured and predicted values at several stages in the logical progression shown in Fig. 1. It is useful to differentiate between the two distinct purposes of these results: material behavior estimates are used to identify significant processes and parameters that require additional testing support; performance estimates for waste forms and EBS materials are used iteratively to identify changes to the EBS design and materials selection that would improve performance model predictions and repository performance under the applicable and relevant environmental conditions of the repository.

22.2 Estimates of the performance of the EBS materials used for geologic disposal consider time scales over much longer time periods (orders of magnitude) relative to the length of time tests are conducted to develop the models and determine model parameter values. In some cases, (for example, corrosion of stainless steels), repository performance calculations will be made using material behavior models based on a range of future environments.

22.2.1 If appropriate analogs are available, however, the models are used to interpolate between existing data in order to estimate the materials behavior. Since precise matches of analog compositions are unlikely, models must also serve to extrapolate or, preferably, interpolate data against material composition in these instances. The intent of using analog materials is to increase the confidence in the performance estimates; 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 performance estimates when they are based on interpolations of available data.

22.3 *Post-Closure Performance Time*—Repository performance for the post-closure period requires calculations to represent the effects of credible features, events, and processes on material alteration over very long times (for example, 10 000 years and longer).

22.3.1 For some process models, the effect of time on material alteration behavior will occur through changes in the environmental conditions that are variables in the model, such as temperature, pH, and solution chemistry, rather than being an independent variable.

22.3.2 Modelling may also require the evaluation of interactions between various materials in the repository system. Some of these interactions may be taken into account through variables that are included in behavior models of the individual materials while other interactions may require additional variables or expanded ranges of values. For example, the dissolution of high-level waste glass and concrete EBS components will likely cause an increase in the pH of groundwater contacting the steel waste package components to values higher than expected for local groundwater. If the model for steel degradation has a pH-dependence term, then the range of pH values for which the steel degradation model is supported should include the higher pH values expected to be generated by glass or cement degradation.

22.3.2.1 Reactions between the breached EBS barrier materials and the ground water may continue to be important over time because the resulting modification of the ground water composition may affect the alteration of spent fuel and glass.

23. Environmental Conditions

23.1 It is recognized that environmental conditions to which materials will be exposed in the repository may change after emplacement. Estimates generated from most materials behavior models will depend on the environmental conditions that are considered, since most models will include dependencies on temperature, groundwater chemistry, etc. For some behavior models, the change in the environmental conditions will be the primary effect of time on material alteration. The performance of the EBS materials should be evaluated for the relevant environmental conditions and, as appropriate, alternative environmental conditions for low-probability scenarios should also be evaluated.

23.2 The time dependence of each environmental variable, for example, temperature, groundwater composition, humidity, mechanical loading, etc. can be used as an input variables for materials behavior models to represent the material performance as the repository conditions change. Which variables are included in a particular model is determined during development of each model.

23.3 Particular attention should be paid to mutually exclusive repository conditions to avoid unrealistic environmental conditions. For example, materials alteration would be predicted to be rapid in liquid water at a high temperature (for example, above 100°C); however, if the repository is porous and thus incapable of maintaining pressurization, these two elements are mutually exclusive.

24. Uncertainties in Model Estimations

24.1 *General Treatment of Uncertainties*—There will be inherent uncertainties associated with characterizing and modeling long-term behavior of materials that provide barriers to radionuclide release under the disposal environment(s). Estimating the confidence in the long-term behaviors predicted for these materials requires identifying the sources of uncertainties in each process-type alteration model and how they are represented in performance assessments. Quantification of these uncertainties is most important for those process models that contribute significantly to the model predictions. This could be done, for example, by first sampling from a probability distribution of parameter values for each material alteration model used to calculate the overall repository performance. Uncertainties for each parameter value could then be statistically propagated to derive a quantitative estimate of the overall uncertainty in the calculated performance. The use of alteration models developed to provide reliable estimates of material behaviors over long time periods will be strongly dependent on the uncertainties in those models. Model uncertainty can originate from uncertainties in the conceptual models, their mathematical representations, and the data used to determine the dependencies on the variables. Uncertainties in the mathematical model arise from the simplifying assumptions and approximations used in formulating the mathematical form of the model and the environmental dependencies. Uncertainties in the conceptual model arise from the incomplete understanding of the processes that contribute to the material behavior and long-term service conditions. The uncertainties that require consideration may be associated with the following:

24.1.1 Data which the process model is developed to represent.

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

24.1.3 The alteration modes represented by the model,

24.1.4 Materials interaction effects represented or taken into account in the model,

24.1.5 The test data used to identify key variables and parameter dependencies, and

24.1.6 The environmental service conditions.

24.2 *Uncertainty in the Mathematical Form of the Model*—The mathematical form of the model is a source of uncertainty whose significance depends on the particular model. The uncertainty likely decreases as models become more mechanistic and less empirical. Mechanistic models that represent known physical or chemical processes of materials alteration mathematically have less inherent uncertainty than do empirical models that represent measured responses. Fully empirical models may be used as bounding cases, or when mechanistic models are either not available or not practically achievable, but the behaviors predicted using empirical models are considered to have greater uncertainty. For example, a bounding empirical model based on a measured alteration rate could be used with confidence as part of a conservative analysis of EBS performance, but confidence in the accuracy of the estimated performance would be very low.

24.3 *Test Data Uncertainty*—Essentially all data used to develop models will be obtained over short periods of time compared with the repository post-closure time period. Additionally, the accuracy of all test data used to support model development will have limitations that must be factored into any model parameter value derived from that data. This will impact both mechanistic and empirical alteration models.

24.3.1 *Model Parameter Uncertainty*—Model parameter values are generally obtained from test data using data regression techniques. These are often used as coefficient values in a materials alteration model. Alternatively, model parameter values may be based on theory, data from the open literature, expert judgment, or some combination thereof; each approach has associated uncertainty. The uncertainty can be reduced to the extent that the alteration mechanism is understood and represented by the analytical model. Model fitting parameters cannot provide a degree of accuracy to the alteration model that exceeds the accuracy of the test data from which they are derived. For example, if corrosion rates are derived from data with an experimental accuracy of ±10 %, the uncertainty in a fitting parameter based on those rates, such as the temperature dependence, will be ≥ ±10 %

24.3.2 *Propagation of Data Uncertainties*—The combined uncertainties in the data and parameters on which the materials behavior models are based should be evaluated using appropriate statistical techniques. These may include propagation and uncertainty budget approaches.

24.4 *Uncertainties in Establishing Environmental Service Conditions*—Uncertainties in the environmental conditions to which materials will be exposed—including the evolution of those conditions with time and materials interactions—should be evaluated for their contributions to the uncertainty in the modeled performance of the EBS materials. The evolution of the physical/chemical environment over the very long post-closure service time is beyond the scope of this practice, but should be expected to contribute additional uncertainty to the calculated performance.

24.5 *Confidence in Materials Alteration Estimates*—Estimates of materials behavior over short periods are expected to have high confidence levels, since models are expected to reproduce the alteration levels that have been directly observed and on which they are based. Estimates for longer periods of time have lower confidence levels. However, confidence in model results will also depend on the particular repository conditions under consideration and the selection of EBS materials.

24.5.1 The selection of EBS barrier materials could be influenced by the level of confidence they provide to the model for the expected primary degradation mode/mechanism. For example, greater confidence in the degradation model for a less corrosion resistant material X compared to the model for more highly corrosion-resistant candidate materials may justify incorporating material X as a "corrosion allowance" into the barrier design.

24.6 *Confidence with Respect to Excluded Alteration Mechanisms*—The high-level nuclear wastes to be disposed in a repository may consist of many different types of waste forms: several kinds of commercial light water reactor spent fuel assemblies; engineered high level radioactive waste glasses, glass-ceramics, ceramics, alloys; Pu immobilized in glass or ceramics; and several hundred distinct forms of non-commercial and test reactor spent fuels. It is not practical to develop alteration models for all waste form types. It is expected that the alteration mechanisms for several waste forms will be similar enough to the alteration model developed for a waste form that has undergone appropriate testing and thus can be applied to other waste forms by assuming the same degradation processes are operative. It is possible that an alteration mechanism that was not observed in the testing of one waste form could significantly contribute to the alteration of a different waste form under long-term repository conditions. An emphasis on the mechanistic understanding of potential alteration modes, careful selection of representative materials for testing, and appropriate characterization and accelerated tests should minimize the possibility that a significant alteration mode will be overlooked or unduly discounted when developing the alteration models. Using materials representing the range of waste form for Confirmation testing (see Section 25) would add confidence that no reasonably probable alteration mode has been overlooked.

24.7 *Uncertainty in Performance Assessment*—Probabilistic performance assessment sometimes use a bounding or conservative approach. The bounding approach uses a worst case value from a range of uncertain values. The conservative approach is not worse case and adopts conservative values rather than using realistic values that may be very uncertain. Both approaches can be incorporated in the uncertainty distribution, if necessary. These two approaches are used as long as the safety objectives of the disposal system continue to be met. Model representations of the degradation processes are generally of a simple form in the performance assessment computer code. This relies, in part, on bounding and conservative approaches for the simplicity but allows the performance assessment results to take the significant uncertainties into account. Thus, the performance assessment can be used to provide information to assist the prioritizing the need for investigation and understanding of the performance of EBS materials.

PERFORMANCE CONFIRMATION

25. Scope

25.1 *Performance Confirmation Requirements*—During the pre-closure or operational period for a geologic repository, which is anticipated to last for decades prior to permanent closure of the facility, it is expected that additional data concerning the long-term behavior of EBS materials will be obtained through confirmation testing. Confirmation tests are intended to provide confidence in the models developed to represent the performance of the EBS materials during the post-closure period. The confirmation tests will provide additional data to which the process model results can be compared. Confirmation testing should focus on the alteration behaviors of those EBS materials that are most likely to impact the overall repository performance. These key materials can be identified through performance assessment sensitivity analyses, expert judgment, analysis of natural analog materials, etc. The performance assessments should take into account the risk from potential radiation exposure due to releases from the repository based on the inventories of spent fuel and high level waste to be emplaced and their expected waste degradation rates.

25.2 *Performance Confirmation Testing*—Performance confirmation encompasses a continuous, broad-based, technical program of tests, experiments, and analyses conducted to provide the information needed to confirm the design and performance of the repository system during the post-closure period. It is anticipated that confirmation testing would be performed after the initial development of process and performance models and up to the time of permanent closure of the repository.

25.2.1 A program for monitoring the condition of the waste packages may be established at the geologic repository operations area. Waste packages chosen for the confirmation test program must be representative of those to be emplaced in the underground facility.

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

25.2.3 The WPMP should include laboratory experiments that focus on the internal condition of the waste packages. To the extent practical, the environment experienced by the waste packages emplaced within the underground facility (for example, underground research laboratories) during the WPMP must be duplicated in the laboratory experiments.

25.2.4 The WPMP should continue as long as practical.

26. Specific Procedure

26.1 Identify processes and parameters that are important to post-closure performance. Identification should be made based on a risk-informed performance-based (RIPB) approach. RIPB focuses on tests, experiments, and analyses that address

Features, Events, and Processes (FEPs) that are significant to the performance of the EBS materials for the repository conditions.

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

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

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

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

26.6 Monitor performance, perform tests, and collect data.

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

26.8 Recommend and implement appropriate actions if data are outside the established tolerances or limits or deviate from values of the parameters relevant to the expected performance of the EBS materials.

27. Quality Assurance

27.1 This practice covers activities related to the evaluation of the long-term behavior of materials used in the EBS for geological disposal that are subject to the quality assurance requirements defined by national law and regulation.

27.2 All data collection and modeling shall be done under a qualified Quality Assurance Program (QAP) defined by national law and regulation.

27.2.1 The consensus standards such as ANSI NQA-1, ASTM standards, the International Organization for Standardization (ISO), and other standards should be used as guidance or references for data collection and modeling.

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

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

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

27.3.3 Data are traceable when they can be related through an unbroken chain to acceptable reference standards, calibration checks, and parallel experiments using standard reference materials from authoritative sources such as standards bodies and institutional standards organizations.

27.4 Models in the form of computer software must be fully documented as defined by national law and regulation and a software quality assurance plan approved under the QAP governing the activity.

28. Precision and Bias

28.1 The parameter values in the alteration models developed under this practice, when determined using curve-fitting and regression of experimental data from accelerated, characterization, and service condition tests, should reflect the precision and bias limitations of that data. The accuracy of a materials alteration model should not be taken as greater than the precision of the test data from which the model, model parameters, and model parameter values are derived. Statements of precision and bias should be developed for the test data used to support model development and the consequent quantitative performance results from the application of this practice. (See Practices E177, E178, and E583).

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