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Standard Practice Guide for Evaluation of the Long-Term Behavior of Materials Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste¹

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 eriteria, 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

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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.



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 (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 1999⁶

IAEA SSR-5 Disposal of Radioactive Waste – Specific Safety Requirements, International Atomic Energy Agency (IAEA), Vienna, Austria, 2011⁶

IAEA GSG-3 The Safety Case and Safety Assessment for the Predisposal Management of Radioactive Waste, International Atomic Energy Agency (IAEA), Vienna, Austria 2013⁶

SSMFS 2008:37 Swedish Radiation Safety Authority Regulatory Code – General Advice, Swedish Radiation Safety Authority, Stockholm, January 30, 2009⁷

Finland Government Decree (736/2008) on the Safety of Disposal of Nuclear Waste, Radiation and Nuclear Safety Authority in Finland (STUK) Helsinki, November 27, 2008⁸

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 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/.www.finlex.fi/en.

⁹ SeeAvailable Compilation of ASTM Standard Definitions, available-from ASTM Headquarters, 100 Barr Harbor Drive, PO Box C700, West Conshohocken, PA 19428-19428-29593 or www.astm.org.

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.
- 3.2.10 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— (https://standards

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 exeavation. 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 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.



Model Development Steps Testing Support What are the properties and environment? **Problem Definition** (Sections 7-9) Attribute Testing (Section 12) **Environmental Conditions** Selection of EBS Materials What processes are significant? Characterization Testing (Section 13) **Model Formulation** Accelerated Tests (Section 14) (Sections 18–20) Service Condition Tests (Section 15) What conditions can the model represent? **Model Support and Confidence** Service Condition Tests (Section 15) ("validation") Testing of Analogs (Section 16) (Section 21) Confirmation Tests (Section 17) Is the material performing as expected?

FIG. 1 Model Development Steps and Testing Support

Estimating Performance (Sections 22–24)

Performance Confirmation (Sections 25–28)

QA during fabrication
Testing during operations

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.

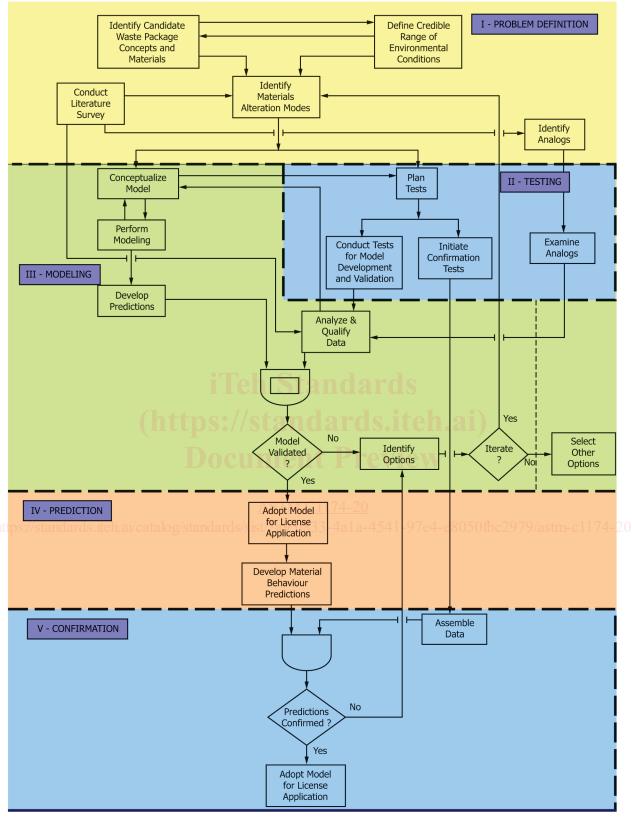


FIG. 2 Logic for the Development of Models for Estimating the Alteration Behavior of Materials

- 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. 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 under-estimated and modeling outputs can be used to provide reliable input to risk-based decision making / optimization. The alteration behaviors of EBS materials having degradation characteristics that are determined to be unimportant to waste isolation do not need to be modelled with the same accuracy and precision as those materials deemed to be important to waste isolation.
 - 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 eonditions.
- 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 eliff-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

rated Tests II en Standards

- 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: