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Standard Practice for
Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste[1]

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1. Scope

1.1 This practice describes test methods and data analyses used to develop models for the prediction of the long-term behavior of materials, such as engineered barrier system (EBS) materials and waste forms, used in the geologic disposal of spent nuclear fuel (SNF) and other high-level nuclear waste in a geologic repository. The alteration behavior of waste form and EBS materials is important because it affects the retention of radionuclides by the disposal system. The waste form and EBS materials provide a barrier to release either directly (as in the case of waste forms in which the radionuclides are initially immobilized), or indirectly (as in the case of containment materials that restrict the ingress of groundwater or the egress of radionuclides that are released as the waste forms and EBS materials degrade).

1.1.1 Steps involved in making such predictions include problem definition, testing, modeling, and model confirmation.

1.1.2 The predictions are based on models derived from theoretical considerations, expert judgment, interpretation of data obtained from tests, and appropriate analogs.

1.1.3 For the purpose of this practice, tests are categorized according to the information they provide and how it is used for model development and use. These tests may include but are not limited to the following:

1.1.3.1 Attribute tests to measure intrinsic materials properties,

1.1.3.2 Characterization tests to measure the effects of material and environmental variables on behavior,

1.1.3.3 Accelerated tests to accelerate alteration and determine important mechanisms and processes that can affect the performance of waste form and EBS materials,

1.1.3.4 Service condition tests to confirm the appropriateness of the model and variables for anticipated disposal conditions,

1.1.3.5 Confirmation tests to verify the predictive capacity of the model, and

1.1.3.6 Tests or analyses performed with analog materials to identify important mechanisms, verify the appropriateness of an accelerated test method, and to confirm long-term model predictions.

1.2 The purpose of this practice is to provide methods for developing models that can be used for the prediction of materials behavior over the long periods of time pertinent to the service life of a geologic repository as part of the basis for performance assessment of the repository.

1.3 This practice also addresses uncertainties in materials behavior models and their impact on the confidence in the performance assessment.

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.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

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

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]

[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.

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

2.2 *ANSI Standard:*[4]

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

2.3 *U.S. Government Documents:*

DOE/RW-0333P, Assurance Requirements and Description, USDOE OCRWM, latest revision

Code of Federal Regulations, Title 10, Part 60, Disposal of High-Level Radioactive Wastes in Geologic Repositories, U.S. Nuclear Regulatory Commission, January 1997[5]

Code of Federal Regulations, Title 10, Part 63, Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada, U.S. Nuclear Regulatory Commission, latest revision[5]

Code of Federal Regulations Title 40, Part 191, Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes, July 2002[5]

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)[6]

3. Terminology

3.1 *Definitions:*

3.1.1 Terminology used in this practice is per existing ASTM definitions, or as understood per the common English dictionary definitions, except as described below.

3.2 *Regulatory and Other Published Definitions*—Definitions of the particular terms below are based on the referenced Code of Federal Regulations, 10 CFR 63 and/or 10 CFR Part 60 which is pertinent to this standard and is under jurisdiction of the Nuclear Regulatory Commission (NRC). If precise regulatory definitions are needed, the user should consult the appropriate governing reference.

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

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

3.2.3 *geologic repository*—a system which is intended to be used for, or may be used for, the disposal of radioactive wastes in excavated geologic media. A geologic repository includes the geologic repository operations area, and the portion of the geologic setting that provides isolation of the radioactive waste.

3.2.4 *important to safety*—refers to those engineered features of the geologic repository operations area whose function is: *(1)* To provide reasonable assurance that high level waste can be received, handled, packaged, stored, emplaced, and retrieved without exceeding regulatory requirements for Category 1 design basis events; or *(2)* To prevent or mitigate Category 2 design basis events that could result in doses equal to or greater than the regulatory values to any individual located on or beyond any point on the boundary of the site.

3.2.5 *important to waste isolation*—refers to those engineered and natural barriers whose function is to provide reasonable assurance that high-level waste can be disposed without exceeding the regulatory requirements.

3.2.6 *high-level radioactive waste, (HLW)*—includes spent nuclear fuel and solid wastes obtained on conversion of wastes resulting from the reprocessing of spent nuclear fuel and other wastes as approved by the NRC for disposal in a deep geologic repository.

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

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

3.2.9 *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 work.

3.2.10 *scientific investigation*—any research, experiment, test, study, or activity that is performed for the purpose of investigating the material aspects of a geologic repository, including the investigations that support design of the facilities, the waste package and performance models.

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

3.2.12 *risk-informed*—refers to an approach to the licensing of a geologic repository based on the understanding that some risk will always exist and that the engineered barrier system and natural barrier system are designed to perform such that the risk is acceptable.

3.2.13 *risk-significant*—pertaining to an engineered barrier system material that has been determined to have a significant effect on the performance of the repository during the regulatory compliance period after closure.

3.2.14 *boundary dose risk*—the quantitative estimate of the expected annual dose to an individual at the repository site boundary over the compliance period weighted by the probability of occurrence. **(10 CFR 63.113)**

3.3 *Definitions of Terms Specific to This Standard:*

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

[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, Mail Stop: SDE, Washington, DC 20401, http://www.access.gpo.gov.

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

3.3.2 *accelerated test*—a test that results in an increase in the rate of an alteration mode or in the extent of reaction progress, when compared with expected service conditions. 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*—any change in the form, state, or properties of a material.

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

3.3.5 *alteration mode*—a particular form of alteration, for example, dissolution or passivation.

3.3.6 *analog*—a material, process, or system whose composition and environmental history are sufficiently similar to that anticipated for the materials of interest to permit use of insight gained regarding its condition or behavior to be applied to a material, process, or system of interest.

3.3.7 *attribute test*—a test conducted to provide material properties that are required as input to behavior models, but that are not themselves responses to the environment. Examples are density, thermal conductivity, mechanical properties, radionuclide content of waste forms, etc.

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

3.3.9 *bounding model*—a model that yields values for dependent variables or effects that are expected to be either always greater than or always less than those expected for the variables or effects to be bounded.

3.3.10 *characterization test*—in high-level radioactive waste management, any test or analysis conducted principally to furnish information used to determine parameter values for a model or develop a mechanistic understanding of alteration. Examples include polarization tests, solubility measurements, etc.

3.3.11 *confirmation test*—a test in 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 the predictions of that model for model validation.

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

3.3.13 *empirical model*—a model based only on observations or data from experiments, without regard to mechanism or theory. An empirical model may be developed from a direct fit of the experimental data such as a regression analysis or may be developed as a model which encompasses all the observed data points; that is, a bounding model.

3.3.14 *extrapolation*—the act of predicting long-term material behavior beyond the range of data collected by empirical observation in short-term tests.

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

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

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

3.3.18 *mechanistic model*—model derived from accepted fundamental laws governing the behavior of matter and energy. It corresponds to one end of a spectrum of models with varying degrees of empiricism.

3.3.19 *pyrophoric*—capable of igniting spontaneously under temperature, chemical, or physical/mechanical conditions specific to the storage, handling, or transportation environment

3.3.20 *semi-empirical model*—a model based partially on a mechanistic understanding and partially on empirical fits to data from experiments.

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

3.3.22 *model validation*—the process through which model predictions are compared with independent measurements or analyses to provide confidence that a model accurately predicts 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 predict alteration behavior under conditions or durations that have not been tested directly. An alteration model that has been demonstrated to provide bounding results under all credible environmental conditions, and is used to provide bounding values for the alteration behavior, may be regarded as validated for its intended usage.

4. Summary of Practice

4.1 This practice covers the general approach for proceeding from the statement of a problem in prediction of long-term behavior of materials, through the development, validation, and confirmation of appropriate models, to formulation of actual predictions.

5. Significance and Use

5.1 This practice supports the development of materials behavior models that can be used to predict alterations in materials over the very long time periods pertinent to the operation of a high-level nuclear waste repository; periods of time much longer than can be tested directly. Under the very extended service periods relevant to geological disposal—much longer periods than those encountered in normal engineering practice—equilibrium or steady state conditions may be achieved and models for reaction kinetics may be replaced by models, if justified, describing equilibrium extents of alteration. This practice is intended for use for waste form materials and materials proposed for use in an EBS that is designed to contain radionuclides released from high-level nuclear waste forms as they degrade over tens of thousands of years and more. Various U.S. Government regulations pertinent to repository disposal in the United States are as follows:

5.1.1 Public Law 97–425, the Nuclear Waste Policy Act of 1982, provides for the deep geologic disposal of high-level radioactive waste through a system of multiple barriers. The radiation release limits are to be set by the U.S. Environmental Protection Agency (EPA) (40 CFR 191). Licensing of such disposal will be done by the U.S. Nuclear Regulatory Commission (NRC).

5.1.2 The analyses described in this Standard Guide can be used to support the demonstration of compliance of the EBS components and design to the applicable requirements of 10 CFR 60 (pertaining to any HLW repository in the U.S.) and 10 CFR 63 (pertaining to the planned HLW repository at Yucca Mountain, NV).

5.1.2.1 10 CFR 60.135 and 60.113 require that the waste form be a material that is solid, non-particulate, non-pyrophoric, and non-chemically reactive, and that the waste package contain no liquid, particulates, chemically reactive or combustible materials and that the materials/components of the EBS be designed to provide – assuming anticipated processes and events - substantially complete containment of the HLW for the NRC-designated regulatory period.

5.1.2.2 10 CFR 63.113 provides that the EBS be designed-such that, working in combination with the natural barriers, the performance assessment of the EBS demonstrates conformance to the annual reasonably expected individual dose protection standard of 10 CFR 63.311 and the reasonably maximally exposed individual standard of 10 CFR 63.312 , and shall not exceed EPA dose limits for protection of groundwater of 10 CFR 63.331 during the NRC-designated regulatory compliance period after permanent closure.

5.1.3 The regulations of the U.S. Environmental Protection Agency (EPA) in Part 191 of Title 40 of the CFR provide that cumulative releases of radionuclides from the disposal system—this refers to the total system performance not just the EBS performance—for the regulatory compliance period after disposal shall have a likelihood of less than one chance in ten of exceeding the values stated for each radionuclide in the regulation. These environmental standards relate to the overall system performance of a geologic repository and they are referred to in NRC requirements of 10 CFR 60.112 and 63.111. Analyses of overall repository system performance may include anticipated and unanticipated events.

5.2 The current governing regulations are 10 CFR 60 as applicable to generic requirements for a repository in the US and 10 CFR 63 as applicable to the proposed repository site at Yucca Mountain. Other site-specific regulations may be required in the development of any alternative or additional US geologic repository site (per 10 CFR 60).

5.3 This practice recognizes that technical information and test data regarding the actual behavior of waste forms and materials that are used in the EBS and exposed to repository conditions for such long periods of time will not be sufficient to develop fully validated models in the classical sense. Rather, the (necessarily) short-term test data acquisition, and use of the data in formulating reliable long-term predictive models, is to be used to support the design, performance assessment, and even the selection of waste package/EBS materials (e.g., low confidence in a degradation model may justify the selection of alternative EBS barrier materials).

5.4 This practice aids in defining acceptable methods for making useful predictions of long–term behavior of materials from such sources as test data, scientific theory, and analogs.

5.5 The EBS environment of interest is that defined by the natural conditions (for example, minerals, moisture, biota, and mechanical stresses) as modified by effects of time, repository construction and operations, and the consequences of radionuclide decay, for example radiation radiation damage, heating., and radiolytic effects. Environmental conditions associated with both anticipated and unanticipated scenarios should be considered.

6. General Procedure

6.1 *Development of Modeling Approach:*

6.1.1 Fig. 1 outlines the logical approach for the development of models for the prediction of the long-term behavior of waste form and EBS materials in a repository. The major elements in the approach are problem definition, testing, modeling, prediction, and confirmation. It is not expected that Fig. 1 will apply exactly to every situation, especially as to the starting point and the number and type of iterations necessary to obtain validated alteration models. However, it is likely that development of models will contain these major elements. Details on these elements are given in Sections 7 – 26. Development of predictive models will likely be conducted under a quality assurance program as discussed in Section 27. An important aspect of predictive models is determination of the uncertainty of the model , including uncertainties in the form of the model (that is, how well the model represents the physical system or process), uncertainties in the data used to determine model parameters, uncertainties in the predicted environmental service conditions to which the model is applied, etc. The consequences of these uncertainties with regard to the performance of the disposal system are used to determine the risk.

6.2 *Identification of Risk-Significant Waste Form and EBS Material Behavior Characteristics:*

6.2.1 Using a risk-informed approach to repository performance assessment, those waste form and engineered barrier materials behavior characteristics that may substantially contribute to risk (by affecting the release of radionuclides from the repository over the regulatory compliance period) are included in the final performance assessment. However, the repository operator must perform initial performance assessments to analyze the sensitivity of specific materials alteration processes to fully identify those barriers that are important to safety and those barriers that are important to waste isolation. It is the long-term behavior of these risk-significant materials that is the subject of this procedure. Criteria for identifying materials that may be risk-significant are the following:

6.2.1.1 Materials, systems, structures, components, and barriers that are depended on to contain the waste form within the repository environment,

6.2.1.2 Materials, systems, structures, components, and barriers that are deployed to protect the containment of the waste form, and

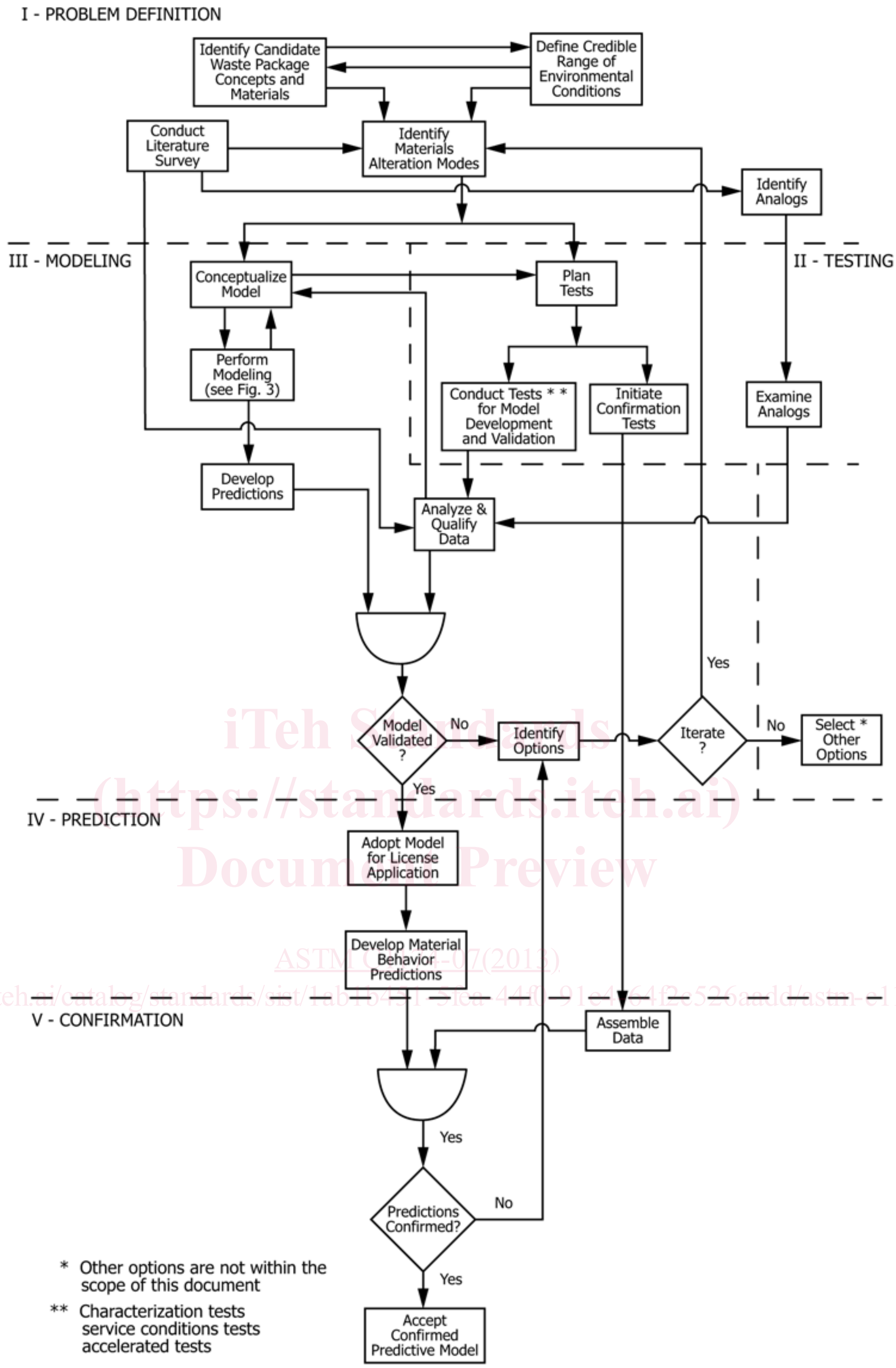

FIG. 1 Logic for the Development of Predictive Models for the Post-Closure Behavior of Waste Package Materials

6.2.1.3 Natural barriers that hold up release of waste radionuclides in the event of containment material failure and waste form degradation.

6.2.2 EBS and waste form materials whose degradation characteristics are determined to be unimportant to waste isolation should be evaluated to determine their useful lifetimes and expected performance, but their behavior models may not need to be as mechanistically based as those important to waste isolation.

6.3 *Identification of Credible Ranges for Environmental Conditions:*

6.3.1 The 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 the effects of EBS components. For example, corrosion of EBS materials and radiolysis will significantly alter the chemistry of the groundwater that contacts the waste forms. The anticipated range of repository environments should be defined and validation of model predictions be done over this range. Tests conducted under conditions outside this range could serve as accelerated tests.

PROBLEM DEFINITION

7. Scope

7.1 Problem definition includes evaluation of the following issues that are important in the development of models to support predictions of long-term behavior of repository materials:

7.1.1 Identification of potential environmental conditions to which the materials may be exposed,

7.1.2 Identification of possible waste-package design concepts,

7.1.3 Identification of waste package materials, including waste forms,

7.1.4 The identity, composition, and condition of the waste forms and important radionuclides,

7.1.5 Identification of potential materials alteration modes,

7.1.6 Identification of appropriate natural analog materials, and

7.1.7 Literature surveys and other sources of information helpful in characterizing the alteration of EBS and waste package materials.

7.2 The objective of the problem definition approach is to identify the processes and interactions that should be included in the predictive model and possible alteration modes. This information is used to design conceptual models and design tests to develop and evaluate process models.

7.3 In this practice, methods are recommended for the development of predictive models for long-term alterations of EBS and waste package materials, including waste forms, 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.

7.4 This practice outlines a logical approach for predicting the behavior of materials over times that greatly exceed the time over which direct experimental data can be obtained. It emphasizes accelerated tests and/or 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. For purposes of this practice, site characterization includes the identification of likely impacts of the environmental conditions on the behaviors of the waste form and 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, and colloid content may be needed to account for changes in the environmental conditions that occur over time.

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

8.3 *Materials Identification*—From the initial concepts and investigations of a repository site, candidate EBS and waste package 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/or the long-term alteration of these and waste form materials in the repository environment.

8.3.2 The selection of WP/EBS materials for waste package and/or EBS application, or the way in which waste forms are configured within a waste package, could also be influenced by the level of validation attainable for the degradation rate model. 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/or 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 in the anticipated temporal and spatial variability in the environmental condition, etc. The waste forms themselves will likely have to be described by ranges to take into account differences in properties due to variations in composition production history, product usage, process control, etc.

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 making