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ENGINEERED BARRIER SYSTEMS PERFORMANCE ASSESSMENT CODES DEVELOPMENT PLAN

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FIGURES

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1 BACKGROUND

This document presents a plan for developing a suite of analyses and codes for assessing in detail the performance of the Engineered Barrier System (EBS). The suite of analyses and codes is collectively called Engineered Barrier System Performance Assessment Codes (EBSPAC). This plan is intended to serve as a guide for the early stages of EBSPAC development. Because of the complexity of Engineered Barrier Subsystem performance assessment, it would be impossible to define *a priori* the exact form each model and analysis would take and even all the models that must be considered. The list and relative priorities will, of necessity, evolve over time as understanding increases.

The engineered barrier subsystem performance requirements consist of two parts:

- a "containment" requirement for high-level waste (HLW) packages
- a radionuclide release rate limit from the engineered barrier subsystem.

These two requirements are intended to control the release of radioactive materials to the geologic setting and to add confidence that the overall system performance objectives for the repository will be met. Specifically, U.S. Code of Federal Regulations (CFR) Title 10 Part 60.113 states the performance requirements for the EBS as follows:

> "The engineered barrier system shall be designed so that assuming anticipated processes and events: (A) Containment of HLW will be substantially complete during the period when radiation and thermal conditions in the engineered barrier system are dominated by fission product decay; and (B) any release of radionuclides from the engineered barrier system shall be a gradual process which results in small fractional releases to the geologic setting over long times . . . ."
>
> "In satisfying the preceding requirements, the engineered barrier system shall be designed, assuming anticipated processes and events, so that: (1) Containment of HLW within the waste packages will be substantially complete for a period to be determined by the Commission taking into account the factors specified in 60.113(b) provided, that such period shall be not less than 300 years nor more than 1,000 years after permanent closure of the geologic repository; and (2) the release rate of any radionuclide from the engineered barrier system following the containment period shall not exceed one part of 100,000 per year of the inventory of that radionuclide calculated to be present at 1,000 years following permanent closure, or such other fraction of the inventory as may be approved or specified by the Commission; provided, that this requirement does not apply to any radionuclide which is released at a rate less than 0.1 percent of the calculated total release rate limit. The calculated total release rate limit shall be taken to be one part in 100,000 per year of the inventory of radioactive waste originally emplaced in the underground facility, that remains after 1,000 years of radioactive decay."

In order to demonstrate compliance with 10 CFR 60.113, it is necessary to develop computer codes to simulate the key processes influencing performance of the EBS. PANDORA (O'Connell et al., 1989) and AREST (Engel et al., 1989) are two computer codes developed and used by the U.S. Department of Energy (DOE) as major computational tools for EBS waste package design and performance assessment. The U.S. Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA) are currently developing a Source Term Code (SOTEC) for calculating the source term from EBS for use in Iterative Performance Assessment (IPA) Phase II.

As described by Ramspott (1988), PANDORA-1 is composed of seven coupled process modules. These are the radiation, thermal, mechanical, environmental (flow of water), corrosion, wasteform alteration, and radionuclide transport modules. O'Connell et al.(1989) state that a model of diffusive contact and transport is deferred to the second phase, PANDORA-2.

The AREST Code, a probabilistic source-term code for waste package performance analysis, was originally developed by the Pacific Northwest Laboratory (PNL) for the Basalt Waste Isolation Project (BWIP) (Liebetrau et al., 1987). The AREST code is divided into three parts:

- Waste Package Containment,
- Waste Package Release, and
- Engineering System Release Components.

A computer Code User's Guide was published in May 1989 (Engel et al., 1989). However, the version of the AREST Code documented in this User's Guide corresponds to the AREST model reported in 1987 by Liebetrau. In 1989, Engel reported that some new features have been incorporated into the AREST Code. The new features include a new release model for a partially saturated media and uranium precipitation. The new release model calculates steady-state release based on rates of matrix dissolution, diffusion, and convection. Engel also states that future developments for the AREST Code will consist of a spatial variability of the repository and additional models for corrosion and release.

The DOE has developed EBS subsystem assessment capabilities. However, the NRC has a requirement to assess DOE compliance with the EBS regulatory requirements set forth in 10 CFR 60.113. To this end, the NRC has a need for a methodology suitable for independent assessment of EBS performance. The SOTEC code and EBSPAC are intended to provide the NRC with that needed methodology. Although the purpose of the document is to describe planned development of EBSPAC, SOTEC is also discussed to some extent because of the integrated nature of the two efforts. Development of SOTEC is separately addressed and funded as part of the IPA study.

2 TECHNICAL APPROACH

Performance Assessment (PA) for the EBS is comprised of two parts: (i) a quantitative estimation of engineered barriers performance through the use of integrated but simplified predictive models, and (ii) detailed auxiliary modeling to support and evaluate the data, assumptions, and modeling approaches used to obtain the simplified quantitative models which predict performance. The two-part approach is dictated by the requirements of performance assessment calculations. On the one hand, we need to have complete and defensible models for each aspect of performance and to include all important anticipated processes and events. At the same time, we require a code or codes which will execute, within reasonable time periods, on currently available computers in a robust fashion consistent with uncertainty propagation.

These competing requirements are particularly challenging in the area of engineered barriers where there is frequently no general agreement upon the governing equations which can be used to predict performance. For example, localized corrosion has been studied in detail for over 30 years, and we still do not fully understand when and how it occurs. Spent fuel or glass dissolution with associated release of radionuclides represent equally problematic areas.

In recognition of the complex requirements of PA, two classes of models will be developed. SOTEC refers to the integrated simplified model that will be used for performance calculations applied to regulatory limits. It is being developed within the PA Program Element in support of the IPA study. EBSPAC refers to the auxiliary models that consider each process in more detail and that provide support to the simplifications required in SOTEC.

The integrated simplified SOTEC will be run in a probabilistic format under the executive module developed for the total system PA code (Sagar and Janetzke, 1991). This format will eliminate duplication of effort and provide greater support for the probabilistic and graphical post processing aspects of the code by sharing the development work from other projects. The executive module currently incorporates Monte-Carlo methods for uncertainty propagation, but is theoretically consistent with other uncertainty/sensitivity methods such as Fast Probabilistic Performance Assessment (FPPA) (Figure 2-1).

EBSPAC, the second portion of model development, is the suite of detailed supporting models which provide the technical basis for the simplified performance models. The suite of supporting codes will be more variable and can range from existing codes (e.g., EQ3/EQ6) to new codes which implement alternative approaches to the problem. This portion of the work recognizes that the DOE methods in a license application cannot be properly evaluated without consideration of alternative models and modeling approaches. The recommended way to determine if the DOE has included all important processes in the analysis is to aggressively investigate poorly understood processes and interactions (e.g., galvanic corrosion) to evaluate their potential significance. Uncertainties and sensitivities in the supporting codes can be estimated with innovative methods such as FPPA or more traditional methods such as Monte Carlo analysis. As more information is gained, the insights from the detailed models will be incorporated into the performance assessment algorithms in SOTEC under the auspices of the PA Program Element. In some situations, EBSPAC modules may be directly exercised with the total PA executive module (Figure 2-1).

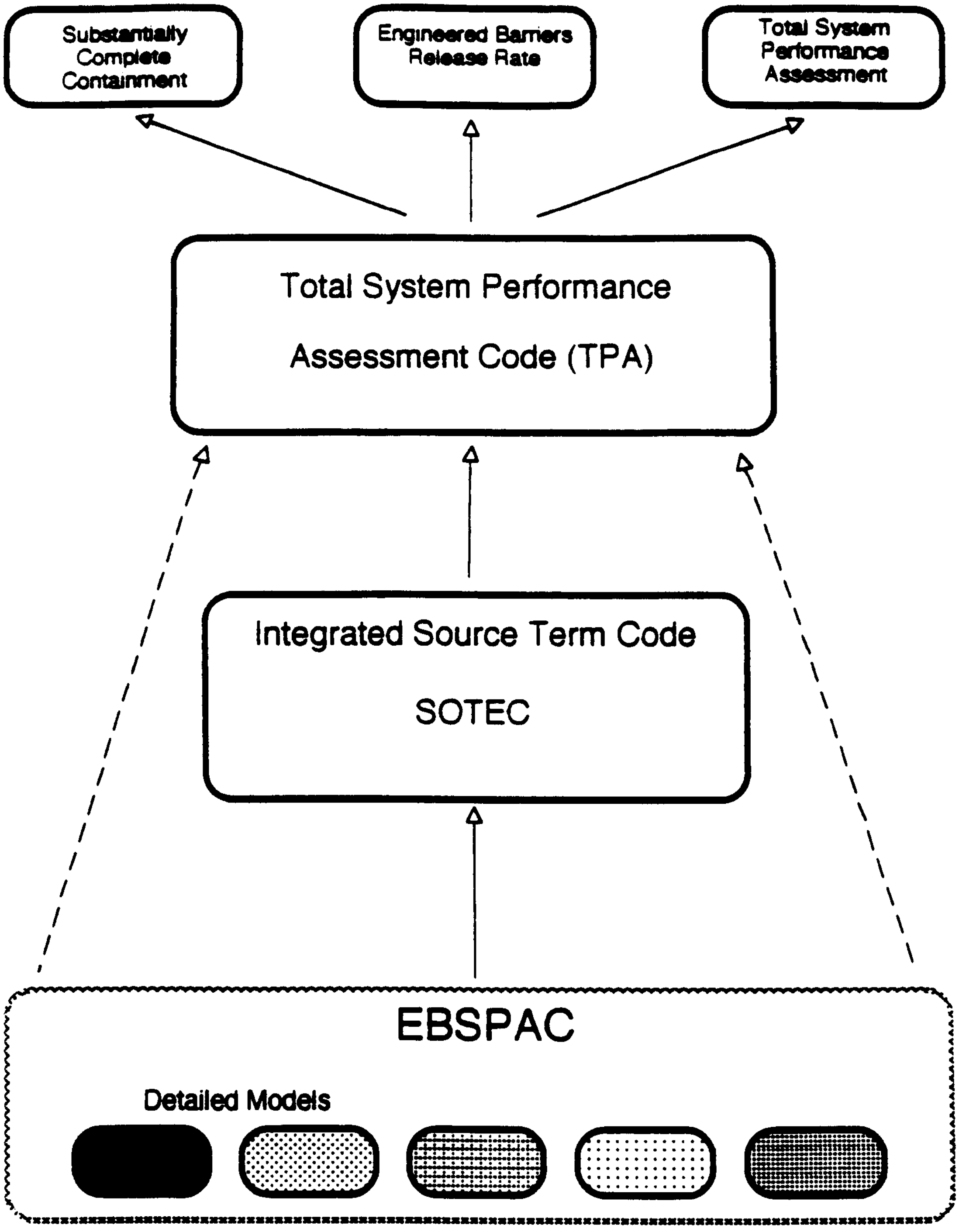

Figure 2-1. Schematic of EBSPAC and relationship to other PA codes

The overall development and implementation of EBSPAC will be in accordance with the CNWRA quality assurance and computer code configuration management requirements.

3 EXAMPLES OF PROCESSES TO BE CONSIDERED IN EBSPAC

The discussion below and the discussion in Manaktala and Interrante (1990) represent examples of the types of processes and models that will be considered to evaluate engineered barriers performance. The list is not comprehensive and will change as understanding evolves. Each heading may include one or several models.

The models described in this section address the performance requirements described below.

- Containment Performance — 10 CFR 60.113(a)(1)(i)(A) and 10 CFR 60.113(a)(1)(ii)(A)

For determining compliance with the containment regulation, the models for thermohydraulic and fluid flow during the early part of the repository life, geochemical and radiological environments, various material transformations and corrosion processes (general, crevice, pitting, stress corrosion cracking, and galvanic effects) for the container materials, and mechanical behavior of waste package components are important.

- Gradual Release Performance — 10 CFR 60.113(a)(1)(i)(B) and 10 CFR 60.113(a)(1)(ii)(B)

The important models needed to support the gradual release of radionuclides from the EBS after the containment period include the following: thermohydraulic and fluid flow, geochemical environment, geochemical and mass transport effects of corrosion reactants and products, waste form (glass and spent fuel) dissolution, and mass transport of radionuclides.

- System Performance — 10 CFR 60.112

The EBSPAC models and analyses collectively contribute to the development of the source term for the determination of the overall system performance. Simplified models are developed from the detailed models identified above and are tested for both anticipated and unanticipated processes and events. This part of the work is performed under the SOTEC development of the IPA. An important activity that will assist system performance evaluations, and to a degree the gradual release performance evaluation, is the development of conceptual models for partially failed waste packages.

The selection of models for development as part of the EBSPAC plan is based on the current conceptual design presented in the DOE Site Characterization Plan (SCP) (DOE, 1988). Priorities for the selection of models for evaluation are established on the basis that there are potentially two classes of container materials—namely, three Fe-Cr-Ni alloys and three copper-base alloys. The containers are placed in an oversized borehole with a sufficient air gap to enhance thermal performance in the waste package vicinity. The borehole is also the defined EBS boundary. The site is unsaturated and during a period of time the near field will remain dry as a result of the decay heat from the waste. An attempt has been made to evaluate and develop models in a generic and as broad based manner as possible. It is recognized that the DOE is currently reevaluating its EBS design strategy. Therefore, the plan presented is subject to changes, and the model development priorities will be changed if DOE makes major conceptual changes. From the DOE presentations to date at the various technical and programmatic meetings, the changes contemplated appear to impact only marginally the efforts underway and the planned work for the next eighteen months.

In determining the ranges of applicability of the various models outlined in this plan, anticipated processes and events based on the SCP (DOE, 1988) review were used. It should be recognized that the definition of anticipated processes and events is an ongoing, multi-disciplinary activity. As a result, a continued effort is needed to interact with several technical disciplines and participate in DOE-NRC technical exchanges. The EBSPAC model development strategy has attempted to provide sufficient bounds for the applicability of individual models. In the case where processes and events still unidentified are determined to exist in the future, new models will be needed and the priorities altered for the EBSPAC activities. When a defined scenario needs to be evaluated, a combination of EBSPAC models and SOTEC will be used. The EBSPAC developmental program plans to have significant input on the identification of the various scenarios and/or the processes and events to be analyzed from ongoing IPA and geosciences activities.

3.1 THERMOHYDRAULICS AND FLUID FLOW

Fluid flow around the waste packages and through the repository, in general, plays a primary role in supporting metallic corrosion and mass transport of radionuclides from the waste into and through the surrounding geology. The flow system is significantly complicated by thermal effects. Heat in the waste package and near-field environment is generated by radioactive decay of waste elements and their daughter products and drives many hydrological, mechanical, and chemical processes. Heat transfer through the waste package and near-field media can occur by convection, conduction, and radiation. The heat transfer rate is determined by the ambient conditions and the thermophysical properties of the media involved. Heat transmission and temperature in the waste package near-field are also affected by physical processes, particularly vaporization and condensation of water (Pruess, 1988).

3.2 GEOCHEMICAL EFFECTS OF ELEVATED TEMPERATURES

Elevated temperatures in the near-field environment at Yucca Mountain are expected to lead to a number of important geochemical variations. Rates of alkali feldspar dissolution and growth of secondary phases such as smectite, clinoptilolite, silica minerals, and/or calcite would be accelerated. Volatilization of water will initially tend to purge the dissolved CO_2 affecting solution pH and will ultimately lead to precipitation of "salts" including silica in the near-field dehydration zone (Murphy, 1992). These conditions may create a more corrosive environment for emplaced engineered materials.

3.3 MATERIAL TRANSFORMATIONS

The waste package can undergo a variety of structural transformations under the repository thermal and environmental conditions. These transformations can affect the performance of the waste package materials either through degradation of their mechanical and physical properties or through degradation of their corrosion resistance. For example, container materials made out of type 304 stainless steel may be susceptible to the precipitation of carbides along grain boundaries and concurrent chromium depletion which can reduce their corrosion resistance. Other container materials may suffer from structural changes including grain boundary segregation of deleterious elements in copper, order-disorder transformations in some nickel alloys, and agglomeration of iron-rich particles in some copper alloys. These structural transformations are material specific, and their effects on material performance can be environment specific. For example, precipitation of chromium carbide at the grain boundary of a Ni-base alloy, alloy 600, can cause increased corrosion in acidic environments but may have no effect or even a beneficial effect in neutral or alkaline environments. Some of the key processes and mechanisms that need to be evaluated for the material stability models include:

- Ability to predict structural transformations for various materials as a function of pertinent variables, such as chemical composition and thermal history
- Kinetics of chromium-rich carbide precipitation and the effect of time and temperature on development of chromium depletion zones in Fe-Cr-Ni alloys
- Kinetics of segregation of metalloid elements such as phosphorus and sulfur to the grain boundaries in copper-base alloys.

3.4 GENERAL CORROSION

General corrosion of the waste container sets the background or framework for other important processes such as localized corrosion. The general corrosion model serves two major purposes: (i) as a predictor of overall or "uniform" corrosion, and (ii) to predict the corrosion potential of the waste container. The corrosion potential of the bulk metal is required by all the other corrosion models (e.g., crevice corrosion) as a boundary condition. General corrosion models have been developed by a number of authors including current CNWRA staff (Walton and Sagar, 1988a; Walton and Sagar, 1988b).

3.5 CREVICE CORROSION

Crevice corrosion is considered to be the most important of the localized corrosion processes not only because crevices are unavoidable in engineering structures, but also because crevice corrosion can be a precursor to other degradation processes such as stress corrosion cracking (SCC). Crevices act to concentrate and acidify the environment within them because of poor mixing with the external environment, as well as electrochemical and chemical (e.g., hydrolysis) reactions within the crevices. In the case of the waste containers, crevices can also act to concentrate the environmental species due to purely thermal processes related to heat transfer from the radioactive decay. Such concentration mechanisms due to heat-transfer effects combined with flow disturbances have been observed in tube-tube sheet and tube-tube support plate crevices in nuclear steam generators. A transient finite difference model for initiation of crevice corrosion based on the work of Watson and Postlethwaite (1990) has been developed at the CNWRA (Sridhar et al., 1991). This model predicts changes in chemical composition of the environment within the crevice as a function of time. Then, a comparison is made at each time period between the calculated chemical composition and the critical chemical composition needed for the crevice to initiate active crevice corrosion. The time at which these two chemical compositions become approximately equal is the initiation time for crevice corrosion. Other models of active crevice corrosion developed by current CNWRA staff (Walton, 1990) can be used to examine phenomena such as repassivation of active crevices. The models need further improvement in terms of considering the effect of temperature, redox species, influence of variable saturation, concentrated electrolytes, and anions other than chloride.

3.6 PITTING

Modeling of pitting is more difficult because the initiation stage is not well defined and initiation sites are often distributed at random on a given surface. Hence, pitting initiation has been modeled using stochastic methods. Stochastic models (Henshall, 1991) have been included in the SOTEC code at the CNWRA to compute pitting corrosion damage function as a plot of number of pits of a particular depth versus depth at increasing time periods to predict penetration of a container. Extreme value statistical methods have been used to predict penetration of pipe walls by pitting, but these depend, for their time-extrapolation, on empirical, short-term data or ad-hoc assumptions of time dependence. Mechanistic models of pitting have been content with predicting the experimental observations of the dependence of pitting on environmental variables. Thus, no satisfactory methods exist for extrapolating short-term pitting corrosion data to long time periods. Because of this limitation and the greater engineering importance of crevice corrosion, less effort will be made on pitting corrosion during the initial EBSPAC development. It must be noted that statistical predictions of pit penetration through the walls of a container can be done using experimental measurements of pit depths in long-term corrosion tests. However, these predictions are again limited to the time frame of the test and can only be used to scale-up in size (i.e., from a small sample to many containers).

3.7 STRESS CORROSION CRACKING

SCC models also need considerable development from the current state of knowledge. Predicting SCC is made difficult by the lack of a single accepted mechanism which is unlike the case of crevice corrosion. The mechanism of SCC has been shown to vary with environment and material. Models, such as the Ford and Andresen model (Anderson and Ford, 1985; Ford and Andresen, 1988), have been developed for crack propagation on stainless steels and nickel-base alloys in high temperature aqueous environments typical of nuclear power plants. However, it is not clear if the same underlying mechanism of SCC is operating for candidate container materials, such as alloy 825 or copper, in the repository environment. Hence, the development of SCC models will be initiated only after significant progress is made in crevice corrosion modeling.

3.8 GALVANIC CORROSION

The waste package will likely be made up of a number of metallic components, potentially including various types of steel, copper, zircaloy cladding, and spent fuel—all in electrical contact. Subsequent to localized breach of the containers, galvanic cells can be expected to form between the different metallic components. These galvanic couplings can lead to pH, potential, and ionic composition dramatically different from expected conditions in the absence of galvanic coupling (Walton, 1991). Differential aeration caused by variable oxygen diffusion rates through partially saturated rock against the container can have similar effects.

3.9 ALTERNATIVE CORROSION MECHANISMS

Several other classes of corrosion may potentially cause problems. Examples are intergranular corrosion, hydrogen embrittlement, hydrogen attack, metallurgical embrittlement, microbially induced corrosion, and dealloying corrosion. In many of these cases, significant research needs to be performed to establish their importance before modeling can be undertaken.

3.10 WASTE FORM DISSOLUTION

A source term release rate model may be based on preferential leaching of certain chemical species or on the gross dissolution of the wasteform or both. The rate of mass transfer is affected by the chemical nature of the soluble material and the solvent, the temperature, and the flow rate of the solvent past the wasteform. The combination of leaching from the wasteform and the dissolution in the liquid phase determines the amount of material available for transport.

Source term models must be developed or adopted for both glass and spent fuel. The models will consider reaction kinetics, thermodynamics, empirical distribution of radionuclides in the waste form, and mass transport. This is an area of primary concern and will be an initial focus area for detailed model development.

3.11 GEOCHEMICAL AND MASS TRANSPORT EFFECTS OF CORROSION REACTANTS AND PRODUCTS

Corrosion products can have a major or even dominant influence on the chemical and physical environment in which release occurs (Walton and Sagar, 1987). For example, steel will more than double in volume as it corrodes to form iron oxides and/or other minerals. The input of iron into the environment and the removal of oxygen can dramatically influence the geochemical environment. For example, subsequent to breach by localized corrosion, the inside of the container may be anaerobic with resulting implications for spent fuel dissolution and mobilization of radionuclides.

3.12 RADIOLYSIS

Radiolysis will influence the geochemical environment in which waste package corrosion and mobilization of radionuclides occurs. Alpha radiolysis may be important in spent fuel dissolution because of its intense localized chemical effects and longevity of alpha emitting radionuclides (Shoesmith and Sunder, 1991). Gamma radiolysis is expected to be most important in influencing corrosion of thin-walled containers.

3.13 MASS TRANSPORT

Mass transport in aqueous or gas phase is important in most aspects of waste package performance including waste form dissolution and corrosion. Mass transport in the aqueous phase may occur by advection and/or diffusion. Transport rates are strongly influenced by colloid formation, solubility constraints, flow rates, and near-field chemistry. Transport in the gas phase is influenced by gaseous diffusion, barometric pumping, pressurization of fuel rods, and generation of helium among other factors. Mass transport will be fully considered in EBSPAC since release of contaminants occurs when radionuclides are transported across the waste package boundary into the surrounding geology, not when the container is penetrated by localized corrosion. Mass transport of corrosion products and reactants along with radionuclide transport will be considered in all models for waste package corrosion and waste form dissolution.

3.14 MECHANICAL STRESS

Mechanical stress in the rock surrounding the waste package and the waste package itself can lead to modifications of the waste package environment including failure. Partial collapse of the borehole or sloughing of rock can lead to development of rock/metal crevices that enhance corrosion. Eventually, mechanical stresses and loss of strength by general corrosion can result in buckling of the waste container.

3.15 PERFORMANCE OF PARTIALLY FAILED WASTE PACKAGES

Most performance analyses of the waste package deal with the system as a simple "or" gate in a fault tree; either the waste package is intact and no radionuclides escape or the waste package has totally failed. Analyses of this type ignore the implications of corrosion products, localized variation in chemical environment, and particularities of the flow system through the partially failed waste package. Without increased understanding and more realistic scenarios, one cannot be certain which scenarios represent overly optimistic assumptions.

3.16 ADDITIONAL CONSIDERATIONS

Once the DOE's Waste Package/EBS design strategy becomes clearer, additional models may be needed to represent new material models or environmental conditions. Technical considerations for containment evaluation were presented by Manaktala and Interrante (1990). Key issues for containment studies were discussed for a variety of repository conditions.

The deliverables and milestones under EBSPAC are included in the FY93-94 Engineered Barrier System Program Element Operations Plan. Future changes on the EBSPAC milestones will be updated, as necessary, by changing pages in the Operations Plan. The results from EBSPAC may be used or modified to supply results relative to the regulatory requirements, both in IPA and in the substantially complete containment example problem.

4 MODEL INTEGRATION APPROACH

EBS analysis will utilize two classes of models, quantitative PA models (SOTEC) and supporting models or analyses (EBSPAC). The models will be applied to three performance measures: (i) Substantially Complete Containment, (ii) Engineered Barriers Release Rate, and (iii) Total System Performance. Integration of all the models and application to the three performance measures is a complex task.

4.1 PERFORMANCE ASSESSMENT CALCULATIONS (SOTEC)

Implementation of the performance assessment models (SOTEC) will occur by integration with the total systems performance assessment code (TPA). The TPA code is made up of four parts (Sagar and Janetzke, 1991): (1) the executive (or manager); (2) algorithm(s) to sample from distributions; (3) algorithms to compute consequences; and (4) algorithm(s) to compute sensitivities and perform uncertainty analyses. The executive of the TPA directs data flow between different parts and controls their execution. SOTEC will be a set of consequence algorithms under control of the executive module. By changing input flags, the executive module can be requested to execute algorithms for any of the desired performance measures such as substantially complete containment, engineered barriers release rate, or total system performance. This approach has the advantage of ensuring a fully integrated approach and avoiding duplication of effort. Parts 1, 3, and 4 of the TPA will be common to all the performance assessments. This provides a much broader base of support for their development. Initially, the TPA code will handle uncertainty with Monte-Carlo simulation. However, the structure of the code is modular and general, allowing incorporation of alternative uncertainty propagation methods such as FPPA. Development of SOTEC will occur under the auspices of the PA Program Element in support of the IPA study. Consideration of anticipated and unanticipated processes and events will be included in SOTEC as part of the IPA.

4.2 SUPPORTING MODELS AND ANALYSES (EBSPAC)

In order to ensure rapid, robust execution and availability, the performance assessment algorithms of SOTEC are anticipated to consist of simplified models. These simplified models must, of necessity, be supported by more complex models and analyses which consider the detailed phenomena controlling performance. As the supporting models are developed and improved, the results will be sequentially incorporated into SOTEC. Anticipated processes and events are within the scope of EBSPAC. Since EBSPAC represents a collection of detailed codes and analyses, there is no general format for covering alternative scenarios. For example, a particular analysis defined within the scope of work for EBSPAC could be an evaluation of alternative scenarios such as climatic change.

EBSPAC represents the recognition that most of the uncertainty in engineered barriers performance assessment lies in the area of limited and inadequate understanding of long-term materials behavior and the complex interactions between different components of the waste package. These types of uncertainty are not amenable to simple quantitative statistical treatment. Instead, significant work must focus on improved understanding of the fundamental processes controlling waste package performance. In order to provide an adequate review of a license application, the NRC must develop the capability to determine both a best estimate of quantitative EBS performance and an understanding of the many processes (e.g., microbial influenced corrosion, galvanic corrosion) which could potentially be of significance to performance but are ignored in current performance assessment codes.

Detailed and supporting codes can take many forms. In the simplest case, a detailed geochemical code (e.g., EQ3/EQ6) could be used to estimate the activity of particular ions around the waste package. A more complex example might be a galvanic corrosion code that attempts to predict galvanic interactions between different corroding metals and the resulting influence on spent fuel dissolution rate and/or the geochemical environment inside the waste package. The output from the detailed code could provide input parameters, assumptions, a response surface, a lookup table, a simplified correlation, or justification for a simplified model in SOTEC.

Detailed supporting models can be used to address questions such as: What is the best model for glass dissolution? Is a simple solubility limited approach adequate for modeling release of some radionuclides? Questions of this type can only be addressed by developing and comparing detailed modeling options.

4.3 UNCERTAINTY/SENSITIVITY ANALYSIS

Uncertainty and sensitivity analysis for SOTEC will be performed by modules in the TPA developed for the PA study. These modules are written in a manner to facilitate modification and incorporation of alternative uncertainty/sensitivity techniques.

In sequential and iterative fashion, computational algorithms and/or modified assumptions from EBSPAC will be incorporated in the simplified algorithms in SOTEC. The decision of when to modify or update a particular algorithm will require comparison of results of simplified algorithms with the results of more detailed or alternative models. Thus, the requirements for sensitivity analysis within EBSPAC differ from the requirements for the IPA and may require different techniques.

One promising statistical method is the Fast Probabilistic Performance Assessment (FPPA) methodology developed by the Center (Wu and Nair, 1988). FPPA is believed to be a viable approach for addressing the assessment needs of the NRC in the EBSPAC development. One of the key features of the FPPA methodology is its capability for providing sensitivity information on the uncertain variables. The sensitivity ranking will be useful in determining whether additional information should be gathered. Based on these results, one can prioritize uncertain variables in an efficient way and compare the sensitivity of different models to the same parameters. The sensitivity information produced by the FPPA approach could provide the NRC with a decision-aiding tool to focus on critical parameters or models and to identify new research areas and guide experimental programs.

5 PLAN OF IMPLEMENTATION

The implementation of the models will be iterative and subject to changes in priority reflecting programmatic and technical considerations, taking into consideration the DOE's program decisions. A primary purpose is to support required performance assessment activities such as IPA and the substantially complete containment example problem that is being conducted under Task 2 of the EBS Program Element. Models and areas of contention identified in the performance assessment tasks will receive increased priority in EBSPAC development.

A second consideration is availability of resources. Clearly NRC cannot duplicate and exhaustively check every aspect of the DOE work. However, selective review with particular emphasis on potentially important processes not fully (or adequately) considered by the DOE is a realistic goal. The proposed schedule represents a best estimate of priorities for the planned resources.

Proposed Schedule:

FY 92

The following deliverables were developed under EBSPAC in FY 92.

Intermediate Milestones	Description	Delivery Date
20-3702-013-305	Preliminary Assessment of Pitting Corrosion Models	9/29/92
20-3702-013-315	TWITCH—A Model for Transient Diffusion, Electromigration, and Chemical Reaction in One Dimension, Version 1.0 MARIANA—A Simple Chemical Equilibrium Module	8/30/92

FY 93

Stress Corrosion Model

Although many mechanistic models of stress corrosion cracking are available in the literature, in which the various atomic and microscopic processes involved in crack initiation and propagation are presented (Gangloff and Ives, 1990), few attempts have been made to develop quantitative models. Most of these quantitative models deal only with the crack propagation stage and are essentially based on the film rupture, slip dissolution and repassivation concepts advanced independently by Scully and Staehle for Fe-Cr-Ni alloys many years ago.

One of the well known models is that developed by Ford and Andresen (Andresen and Ford, 1985; Ford and Andresen, 1988) to predict environmentally assisted crack growth rate for several alloys (304 stainless steel, carbon steels, and Alloy 600) in boiling water reactor (BWR) environments. Crack growth rate is expressed as:

$$\frac{da}{dt} = F(n)\dot{\epsilon}_{ct}^{n} \tag{1}$$

where $F(n)$ is a constant which is a function of n, a parameter that represents the effect of the environment and alloy composition, and $\dot{\epsilon}_{ct}$ is the strain rate at the crack tip. Under constant loading conditions, $\dot{\epsilon}_{ct}$ is proportional to K^4, where K is the stress intensity factor.

The applicability of this model to conditions prevailing in HLW disposal (lower temperatures and more complex environments than BWR water) will be examined, as well as the effect of variations of n, $\dot{\epsilon}_{ct}$ and K on crack growth rate. Alternative formulations of the same conceptual model, such as those developed by Garud (Garud, 1990), will be examined if the parameters needed in this case are more readily accessible.

Since extensive work is needed to establish the validity of these models for the environmental conditions of a HLW repository, only a preliminary assessment of the above described models will be completed and presented during the early part of FY93. The ongoing activity in this area will be a selection and further development of a mechanistic model for numerical purposes.

Crevice and Pitting Corrosion

Existing steady-state and transient crevice corrosion models will be modified to reflect better treatment of chemical reaction. Additionally, the possibility of incorporating activity coefficients for concentrated solutions in the existing crevice corrosion models will be examined. If feasible, this feature will be added to the models and a parametric study will be performed to examine importance.

Release Rate of Radionuclides from Packages Containing Spent Fuel

A detailed analysis will be performed for release rate from waste packages containing spent fuel. The analysis and model will consider processes such as wasteform alteration rate, secondary mineral formation, colloid generation, and mass transport. Mass transport calculations will consider transport through the near field of radionuclides by advection and diffusion with chain decay.

Intermediate Milestones	Description	Planned Date
20-3702-013-355	Assessment of Stress Corrosion Cracking Models	2/15/93
20-3702-013-365	Modification of Crevice and Pitting Corrosion Models with Summary Report	5/01/93
20-3702-013-405	Spent Fuel Dissolution Model and Report	9/25/93

FY 94

Release Rate of Radionuclides from Packages Containing Glass Wasteform

A detailed source term code for glass dissolution will be developed. This code will consider kinetics of glass dissolution, formation of secondary silicate minerals, formation of secondary minerals controlling radionuclide solubility, colloid formation, and mass transport of radionuclides.

Partially Failed Waste Containers

Models will be developed and analyses performed to evaluate performance of partially failed waste packages. Currently, most performance assessment models consider the waste package to be either intact or completely failed. Flow scenarios through the waste package are limited to simplistic idealizations such as a "bathtub" or dripping flow. Without examination of alternative, potentially more realistic failure scenarios, the limitations of the simplistic approach cannot be evaluated. Of greatest concern is the possibility that the simplistic scenarios may not represent a conservative analysis. The work will consider cases such as diffusion through partially saturated corrosion products and rock in the absence of water at atmospheric pressure, limitations on mass transport through localized failures, and variations in chemistry and oxidation/reduction conditions inside the waste package.

Corrosion Potential

A code will be developed to evaluate the influence of variations in wetted area and activity of localized corrosion cavities on the corrosion potential and corrosion rate at the surface of the waste container. This code is to be applied in conjunction with the codes for crevice corrosion initiation and active crevice corrosion along with experimental data collected at the CNWRA to evaluate the hypothesis of cycles of activation and repassivation of crevices related to transient surficial moisture conditions. The code will also estimate the overall corrosion potential and corrosion rate (i.e., general corrosion) of the container.

Intermediate Milestones	Description	Planned Date
20-3702-013-375	Code and Report on Glass Dissolution	1/01/94
20-3702-013-415	Stress Corrosion Cracking Model and Report	2/01/94
20-3702-013-425	Partially Failed Waste Containers Code(s) and Report	7/01/94
20-3702-013-435	Corrosion Potential and Wetted Area Code	9/25/94

6 CONCLUSIONS

Performance objectives set forth in 10 CFR 60.113 contain the requirements for the performance of particular engineered barriers after permanent closure of the repository. To evaluate the conformance of the DOE's EBS subsystem design and performance analyses of these designs to the regulations, the NRC needs a viable tool/methodology that is technically sound and is able to accommodate evaluation of alternate or extreme scenarios. Regulations in 10 CFR 60.113 contain numerical values of performance requirements in terms of times for containment and for gradual release rates. These numerical values dictate the use of computer programs that compute and manage diverse process models in addition to interacting with engineering and research databases. The development plan for the EBSPAC attempts to provide the compliance determination methodology needed in evaluating the performance objectives outlined in 10 CFR 60.113.

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