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PLANNING AND STATUS REPORT ON THE ENGINEERED BARRIER SYSTEM PERFORMANCE ASSESSMENT CODE (EBSPAC) AND SUPPORTING DETAILED ANALYSES

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ABSTRACT

This document describes the planning and status of detailed analyses that will be carried out in support of the engineered barrier system performance assessment code (EBSPAC). The prioritization of the detailed analyses is consistent with the vertical slice approach. The list of Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA) staff coordinators and a brief description of each of the modules are provided. The development of the detailed analyses will also be coordinated with the development of modules in the Iterative Performance Assessment (IPA) Phase 3 activity. However, the modules in the IPA Phase 3 activity are considered to be abstractions of the detailed analyses performed in the EBS program. This planning and status document is intended to be updated periodically and reissued as administrative items.

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INTRODUCTION

The purpose of this document is to describe a plan for conducting the performance assessment of the engineered barrier system (EBS), principally the waste packages and waste form, in relation to satisfying the regulatory requirements for the EBS. In addition, the document describes how such an activity will be coordinated with the total system performance assessment (TPA) activities. This document is intended to be a planning tool and, as such, does not provide detailed descriptions of individual models which are available in other Center for Nuclear Waste Regulatory Analyses (CNWRA) documents. However, a brief description of the various models is provided, along with the names of potential staff members who will be responsible for development of the models and an estimated time frame in which a first iteration of the product is anticipated. It must be emphasized that this list of topics and potential authors is incomplete at the present time and will evolve with the progress of the program.

At present, the two regulatory requirements pertaining to the performance of the EBS as provided in 10 CFR 60.113(a) are:

- Substantially complete containment of high-level waste (HLW) within the waste packages for a period of at least 300 to 1,000 years following permanent closure

- Fractional annual release rate of any radionuclide from the EBS following containment not exceeding 1 part in 100,000 of the inventory of that radionuclide calculated to be present at the end of 1,000 years

Even if the subsystem requirements are deleted by changes in regulations (e.g., in response to the currently released report by the National Academy of Sciences), the defense-in-depth concept and also the assessment of total system performance would require a calculation of the performance of the EBS and the waste package. In addressing the key technical issue (KTI) of waste package degradation, several key technical uncertainties (KTUs) have been identified:

- Prediction of thermomechanical effects on the waste package and the EBS

- Prediction of environmental effects on the waste packages and the EBS

- Prediction of criticality events in waste packages

- Extrapolation of short-term laboratory and prototype test results to predict long-term performance of waste packages and EBS

- Prediction of the evolution of groundwater conditions near and within the EBS (part of the KTI on groundwater in the near field)

- Prediction of release path parameters (such as the size, shape, and distribution of penetrations of waste packages)

- Prediction of the releases of gaseous radionuclides

- Prediction of the release of nongaseous radionuclides

These KTUs form the basis for detailed safety reviews of the license application as described in the Nuclear Regulatory Commission (NRC) License Application Review Plan (LARP) under Sections 5.2 and 5.4.

A two-tiered approach is considered in conducting the subsystem performance assessment. This is illustrated schematically in Figure 1. The detailed analyses, not all of which are indicated in Figure 1, form the basis for judging the adequacy of the more abstracted models that will be used in performance assessment calculations. The detailed analyses can also be used as auxiliary analyses to judge whether a certain phenomenon is important for the EBS performance. The EBS Performance Assessment Code (EBSPAC) will be used to calculate the subsystem performance and will be the source term module in the TPA code. The first version of the EBSPAC code will include features of the existing codes, such as SCCEX and SOTEC.

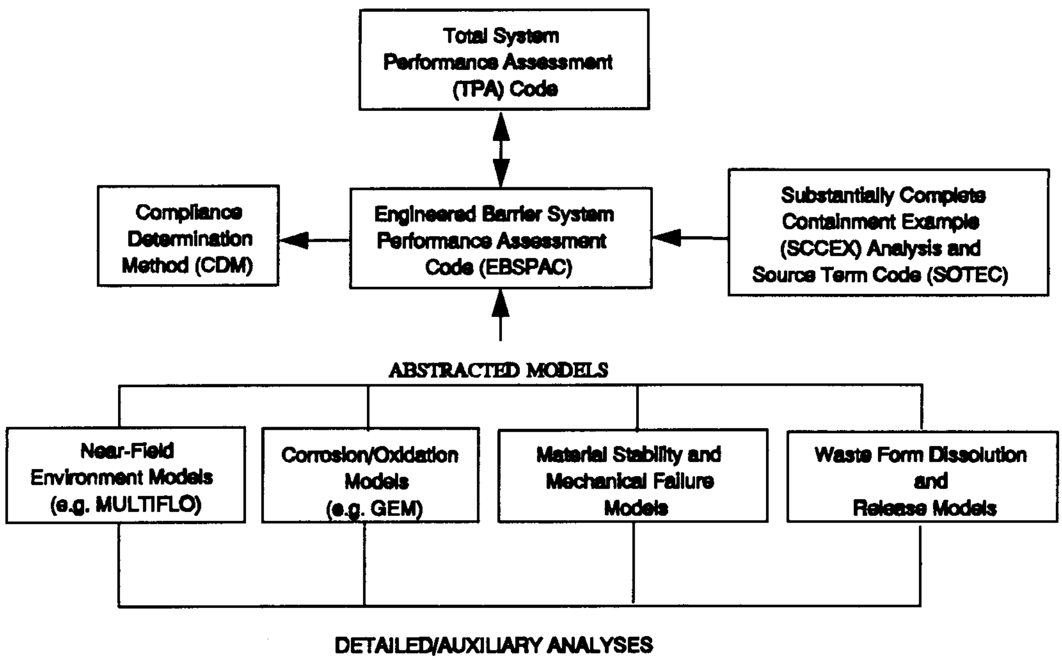

Figure 1. Schematic illustration of the different levels of models

PLAN IMPLEMENTATION

The list of detailed analyses and their present schedule for completion is shown in Table 1. In addition, the plan for EBSPAC code development is shown. The coordinators for the different analysis topics are shown, but the other participants are not listed at present. These names may be added at a later stage as the development of these topics get underway. In some cases, simpler analyses are anticipated at an early stage while more detailed analyses continue to be conducted.

Table 1. Detailed analysis topics, schedule, and coordinators

Main Topic	Subtopics	Coordinator	Tentative Schedule
EBSPAC Code Development and User Manual		PL	FY96
Materials Stability	MPC Weld Material Stability	NS	FY96
	Inner and Outer Overpack Stability	NS	FY97
	MPC Basket Stability and Criticality Control Issues	HM	FY96
Near-Field Environment	Thermohydrologic Effects	PL	FY96* & 97
	Corrosion Product Effects	GC	FY97
	Radiolysis Effects	GC	FY98
	Microbial Effects	GC	FY98
General Corrosion/ Oxidation	Oxidation (dry)	TA	FY96* & 97
	Wet/Aqueous Corrosion	GC	FY96* & 97
Localized Corrosion		GC	FY96* & 97
Stress Corrosion Cracking		GC	FY96* & 98

* A simpler model/analysis will be provided first

TA—Tae Ahn; GC—Gustavo Cragnolino; CI—Charles Interrante; PL—Peter Lichtner; HM—Hersh Manaktala; NS—Narasi Sridhar

Table 1. Detailed analysis topics, schedule, and coordinators (cont'd)

Main Topic	Subtopics	Coordinator	Tentative Schedule
Corrosion Potential and Galvanic Corrosion Effects		NS	FY96* & 97
Hydrogen Effects	C-steel Outer Overpack	CI	FY98
	Corrosion-Resistant Alloy Inner Overpack/MPC	NS	FY98
Radionuclide Release From Spent Fuel	Gaseous Release	TA	FY96* & 97
	Aqueous Release	PL	FY96* & 97
Radionuclide Release From Glass		HM	FY97* & 98
Colloidal Transport of Radionuclides		TA	FY98 & 99
Cladding Performance	Corrosion and Stress Corrosion Cracking	GC	FY97* & 00
	Delayed Hydride Cracking/Creep	HM	FY 00
Radionuclide Release From Partially Failed Waste Packages		TA	FY 00

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Materials Stability:

Materials stability is a function of thermal loading strategy as well as the design of individual waste packages. The consequences of materials instability in combination with mechanical stresses are: (i) fracture of overpacks and multipurpose canister (MPC), especially in the weld regions; (ii) premature intrusion of water increasing the probability of criticality as well as radionuclide release; and (iii) segregation of neutron absorbers and spent fuel increasing criticality. The analyses in this topic will focus on several issues pertaining to materials instability: (i) the high wall temperatures expected for the 21-PWR loaded MPC (currently designed to be made of type 316L stainless steel) may lead to the formation of brittle α' phase in the welds; (ii) the long thermal exposure may lead to segregation of deleterious elements to grain boundaries and result in loss in fracture strength (fracture toughness) of outer carbon steel overpack (temper embrittlement); (iii) the borated materials, proposed to be used as neutron absorbers, may embrittle over time due to either segregation of boron to grain boundaries or formation of embrittling intermetallic phases stabilized by boron. The mechanical loading may arise from either residual stresses due to welding or seismic events. The calculation of the mechanical stresses is not the objective of this task and may be carried out in other programs. The precipitation of embrittling second phases and their effect on the fracture properties (fracture toughness or strength) will be the focus of this activity.

Near-Field Environment:

The near-field environment may be affected by thermohydrological effects (evaporation, dripping from fractures, heat-pipe phenomena), corrosion of overpacks (generation of ferrous and ferric compounds, acidification in cracks or crevices due to hydrolysis of dissolved metal ions), radiolysis (only when the thick overpack is removed by corrosion), "man-made" materials (concrete, hydraulic fluids, diesel, etc.), and microbial processes. Modeling all these rigorously may be unrealistic in the present scope and schedule of the program. Some processes such as the coupled reaction and two-phase flow are being examined using the MULTIFLO code (Lichtner, 1995) to determine the chemistry of the water that could potentially contact the waste package. The crevice chemistry has been examined initially using the TWITCH code (Walton and Kalandros, 1992) and the work will be extended using the GEM code (Lichtner, 1994). The present state of knowledge of microbiological effects does not permit rigorous modeling. The experimental investigations in the research projects may shed some light on environmental parameters that may be important in relation to microbially influenced corrosion (e.g., thiosulfate or sulfide concentration arising from the metabolism of sulfate-reducing bacteria).

General Corrosion/Oxidation:

Uniform oxidation in a dry environment at the anticipated repository temperatures is not considered to be a significant failure mode, even for a carbon steel overpack. However, an empirical rate law for oxidation has been used for both dry oxidation and uniform corrosion in an aqueous medium in the U.S. Department of Energy (DOE) waste package performance assessment (Stahl et al., 1995). The basis for such an equation and alternate rate laws derived from more fundamental mechanistic considerations will be examined in this task. Additionally, the conditions for intergranular oxidation and the rate-controlling processes such as oxygen diffusion along grain boundaries will be investigated. Intergranular oxidation may lead to grain-boundary embrittlement and cracking.

Localized Corrosion:

The repassivation potential concept has already been used in previous waste package performance assessment calculations (Cragnolino et al., 1994). An alternative method of modeling localized corrosion, based on stochastic aspects of pit generation, has been proposed by the DOE (Henshall, 1995). The relationship between these two modeling approaches will be examined. The parameters in the localized corrosion model will be improved by further review of relevant literature and results of the experimental work conducted in the project.

Stress Corrosion Cracking:

The repassivation concept has also been used to determine the occurrence of stress corrosion cracking (SCC) of austenitic stainless steels in chloride solutions (Cragnolino et al., 1994). However, a similar concept may not be applicable to carbon steels. A more detailed technical basis for the use of repassivation potential for SCC is also needed. The experimental investigation in the Engineered Barrier System Experimental Research (EBSER) project will provide the required basis by measuring crack growth rate at potentials above and below E_{rp}.

Corrosion Potential and Galvanic Coupling Effects:

Corrosion potential calculations have been included in previous waste package performance assessments (Cragnolino et al., 1994). Knowledge of the corrosion potential and its evolution with time is essential in estimating both localized corrosion processes as well as uniform corrosion rates. In addition, the advanced conceptual design consists of multiple metals in contact with each other. The effect of galvanic coupling on the corrosion potential of the various components of the waste package will be calculated in this task.

Hydrogen Effects:

Hydrogen embrittlement is one of the possible failure modes of the waste package (Sridhar et al., 1994). Two aspects of hydrogen embrittlement that are of interest are: (i) embrittlement of the carbon steel outer overpack and (ii) embrittlement of the Ni-base alloy inner overpack. Modeling hydrogen embrittlement of these materials was briefly reviewed previously (Sridhar et al., 1994). While the possibility of hydrogen embrittlement cannot be ignored, further development of hydrogen embrittlement models is considered to be a lower priority than that of the localized corrosion and materials stability models. This is because of the low-carbon content of the steel and anticipated temperatures well above ambient temperatures and, therefore, above the ductile brittle transition temperature (DBTT).

Radionuclide Release From Spent Fuel:

Calculating radionuclide release from spent fuel is important not only to provide a source term for TPA but also to determine the technical basis for quantifying substantially complete containment. The gaseous release of ^{14}C has been modeled by Ahn (1994) and van Konynenburg (1994) among others. The aqueous release models continue to be studied by many groups using both chemical leaching and electrochemical dissolution techniques (e.g., Loida et al., 1995; Sunder et al., 1995) accompanied by the identification of the role of secondary mineral phases. A review is ongoing at the CNWRA on the importance of various factors affecting aqueous radionuclide release from spent fuel. This review along with the code GEM will be used to evaluate aqueous radionuclide from spent fuel. Mechanistically based models will be compared with those empirically derived from parametric studies of environmental variables on spent fuel

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dissolution, such as those developed by DOE for UO_2 (Steward and Weed, 1994). The modeling in this area will benefit considerably from the investigations in other projects, notably the near-field processes research project.

Radionuclide Release From Glass:

The dissolution of glass waste form and the resultant release of radionuclides have been reviewed by many authors (e.g., U.S. Department of Energy, 1994). This task will focus on continuing the development of glass dissolution models through a review of literature data.

Colloidal Transport of Radionuclides:

Potential implications of colloids on the radionuclide release from the repository to the accessible environment were recently reviewed along with certain modeling approaches (Manaktala et al., 1995). Further development of an acceptable modeling approach will be undertaken.

Cladding Performance:

The uncertainty in the DOE strategy with respect to cladding credit makes modeling of cladding performance lower in priority than modeling radionuclide release from waste forms. However, cladding performance may be affected either by localized corrosion and/or SCC due to an enriched chloride-containing local environment or by hydride redistribution upon cooling of the fuel under repository conditions.

Release From Partially Failed Waste Packages:

Release from waste package overpacks with through-wall penetrations have been modeled previously (Pescatore and Sastre, 1988). While this analysis was conducted for a single-wall container, modeling the case of multiple overpacks may be important in determining release of radionuclides from the current design of waste packages.

SUMMARY

Various factors affecting the performance of the EBS are outlined in the previous section and a brief description is provided for each of them. The analyses of these factors will proceed according to two schedules: (i) initial, simplified analyses for input to EBSPAC so that the MPC license application as well as the topical report on disposal criticality can be reviewed in FY96 and FY97, and (ii) continued development of detailed analyses in order to attain greater confidence in the simplified analyses. The prioritization of the analyses topics is consistent with the vertical slice approach in the area of waste package degradation. Those topics that directly pertain to the license application review of MPC with respect to disposal issues will be considered first followed by topics related to overall repository performance issues.

REFERENCES

Ahn, T. 1994. Long-term C-14 source term for a high-level waste repository. *Waste Management* 14(5): 393–408.

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Cragnolino, G., N. Sridhar, J. Walton, R. Janetzke, T. Torng, J. Wu, and P. Nair. 1994. *Substantially Complete Containment—Example Analysis of a Reference Container*. CNWRA 94-003. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

Henshall, G.A. 1995. Stochastic modeling of the influence of environment on pitting corrosion damage of radioactive waste containers. *Scientific Basis for Nuclear Waste Management XVIII*. T. Murakami and R.C. Ewing, eds. Pittsburgh, PA: Materials Research Society: 679–686.

Lichtner, P.C. 1994. *Engineered Barrier System Performance Assessment Codes (EBSPAC) Progress Report October 1, 1993, through September 25, 1994*. CNWRA 94-026. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

Lichtner, P.C. 1995. *Multi-Phase Reactive Transport Theory*. NUREG/CR-6347. Washington, DC: Nuclear Regulatory Commission.

Loida, A., B. Grambow, H. Geckeis, and P. Dressler. 1995. Processes controlling radionuclide release from spent fuel. *Scientific Basis for Nuclear Waste Management XVIII*. T. Murakami and R.C. Ewing, eds. Pittsburgh, PA: Materials Research Society: 577–592.

Manaktala, H., D. Turner, T. Ahn, V. Colten-Bradley, and E. Bonano. 1995. *Potential Implications of Colloids on the Long-Term Performance of a High-Level Radioactive Waste Repository*. CNWRA 95-015. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

Pescatore, C., and C. Sastre. 1988. Mass transfer from penetrations in waste containers. *Scientific Basis for Nuclear Waste Management XI*. M.J. Apted and R.E. Westerman, eds. Pittsburgh, PA: Materials Research Society: 773–782.

Sridhar, N., G.A. Cragnolino, D.S. Dunn, and H.K. Manaktala. 1994. *Review of Degradation Modes of Alternate Container Designs and Materials*. CNWRA 94-010. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.

Stahl, D., and J.K. McKoy. 1995. Impact of thermal loading on waste package material performance. *Scientific Basis for Nuclear Waste Management XVIII*. T. Murakami and R.C. Ewing, eds. Pittsburgh, PA: Materials Research Society: 671–678.

Steward, S.A., and H.C. Weed. 1994. Modeling of UO_2 aqueous dissolution over a wide range of conditions. *Scientific Basis for Nuclear Waste Management XVIII*. A. Barkett and R.A. van Konynenburg, eds. Pittsburgh, PA: Materials Research Society: 409–416.

Sunder, S., D.W. Shoesmith, and N.H. Miller. 1995. Prediction of the oxidative dissolution rates of used nuclear fuel in a geologic disposal vault due to the alpha radiolysis of water. *Scientific Basis for Nuclear Waste Management XVIII*. T. Murakami and R.C. Ewing, eds. Pittsburgh, PA: Materials Research Society: 617–624.

U.S. Department of Energy. 1994. *High-Level Waste Borosilicate Glass: A Compendium of Corrosion Characteristics*. DOE-EM-0177. Washington, DC: U.S. Department of Energy.

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van Konynenburg, R.A. 1994. Behavior of Carbon-14 in waste packages for spent fuel in a tuff repository. Submitted for publication in *Waste Management*.

Walton, J.C., and S.K. Kalandros. 1992. *TWITCH—A Model for Transient Diffusion, Electromigration, and Chemical Reaction in One Dimension*. CNWRA 92-019. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses.