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ASSESSMENT OF ENGINEERED BARRIER SYSTEM
AND DESIGN OF WASTE PACKAGES*

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ABSTRACT

The U.S. Nuclear Regulatory Commission has established two post-closure performance objectives for the Engineered Barrier System (EBS) in a geologic repository. These require containment of the waste followed by controlled release. The EBS for a repository in unsaturated tuff at Yucca Mountain is designed to meet these performance objectives. The major components are the waste form, container, air gap, and borehole liner. Assessment of post-closure performance of the EBS is based on allocating performance for various components toward meeting overall design objectives. Because of the unprecedented time periods considered, 1000 to 10,000 years, computer modeling is essential and will be used in conjunction with testing to assess whether the performance allocations are met.

INTRODUCTION

The Nuclear Regulatory Commission (NRC) regulation, 10 CFR Part 60[1], establishes two major performance objectives for the Engineered Barrier System (EBS): assuming anticipated processes and events, the EBS shall be designed to provide substantially complete containment within the waste packages for 300 to 1000 years as determined by the NRC (the containment performance objective) and to provide control of the release

rate from the EBS following the containment period up to 10,000 years (the release control performance objective).

The EBS is defined in 10 CFR 60 as the waste packages and the underground structure, not including shafts and boreholes. The Department of Energy (DOE) has adopted a tentative interpretation of the EBS boundary as the wall of the emplacement hole. That is, the EBS consists of anything inside the emplacement hole. Such a boundary is conservative and simple to define.

Because the containment performance objective in 10 CFR 60.113 is qualitative, the DOE tentatively interpreted "substantially complete containment" in terms of quantitative design objectives in the Site Characterization Plan - Consultation Draft [2]. Following consultation with the NRC, the DOE has prepared a revised interpretation of substantially complete containment that will be released when the statutory SCP is published.

The controlled release performance objective in 10 CFR 60.113 requires that the EBS be designed so that, assuming anticipated processes and events, the yearly radionuclide release rate from EBS following the containment period and extending until 10,000 years after closure shall not exceed one part in 100,000 of the inventory of each nuclide calculated to be present at 1000 years after closure, except that any radionuclide may be released at an annual rate not to exceed one part in 10^8 of the total 1000-year inventory. This unequivocal numerical requirement provides the basis for assessment of the EBS for controlled release.

There are other regulatory requirements placed on the waste package in 10 CFR 60. Section 60.135 requires that individual components or properties not compromise the overall waste package, repository, or site performance. It also sets specific criteria such as requiring solid waste forms and sealed containers. For example, a particulate waste form such as the calcine at Idaho may not be used without further consolidation. Section 60.111 requires up to 50 years retrievability following start of waste emplacement. Although this requirement lies on the "geologic repository operations area," the waste package design must support meeting this requirement.

Section 60.112 requires that the EBS support the overall system in meeting Environmental Protection Agency standards in 40 CFR Part 191.

CURRENT CONCEPTUAL DESIGN

Because of the current interpretation of the EBS as the wall of the emplacement hole, the EBS is virtually synonymous with the waste package. The major EBS components in the current conceptual design for Yucca Mountain are the waste form, a container, an air gap, and a borehole liner. The borehole liner is included to assure retrievability of the waste for at least 50 years, as required in 10 CFR 60.111. At present the liner has no assigned function in containment or release control.

The EBS is being designed to be compatible with and take advantage of the unsaturated zone environment. An explicit design feature of the EBS is engineering the thermal field in the repository to keep a substantial number of waste packages above the local boiling point of water (97°C) for hundreds of years. This will enhance the already dry

conditions expected in the repository. Similarly, the air gap is part of the engineered system and serves a function in an unsaturated site by inhibiting contact of liquid water with the container. These two elements, although nontraditional, are nevertheless part of the Engineered Barrier System design.

The container is the waste package component for which the greatest degree of engineering flexibility exists, and it is a primary barrier for providing substantially complete containment. For a Yucca Mountain repository, the container is based on a corrosion resistance concept. Therefore, it is thinner and lighter than corrosion allowance containers. Approximately 5 m long, 0.7 m diameter, and 1 cm thick, it may be emplaced in either a vertical or horizontal configuration. Selection of the emplacement orientation and of a single metallic material from six currently under consideration is to be completed by September 1989 as input to the Advanced Conceptual Design phase. AISI 304L or AISI 316L austenitic stainless steel, Alloy 825 (40Ni-40Fe-20Cr-Ti stabilized), CDA 715 (70/30 copper-nickel), CDA 613 (aluminum bronze), and CDA 102 (high conductivity copper) are the materials under consideration. A formal process of selection criteria development and review and then selection according to those criteria is currently underway.

The waste forms include both borosilicate glass in stainless steel pour canisters and spent reactor fuel. The glass waste sources are the Defense Waste Processing Facility at Savannah River and the Demonstration Project at the West Valley, N.Y. site. The spent fuel includes both BWR and PWR fuel from U.S. commercial reactors. It may be disposed as either intact assemblies or consolidated fuel rods. Unlike the liner, air gap,

and container, the waste forms are not subject to site specific engineering. Only the glass is a manufactured waste form. Spent fuel does meet the NRC requirements in 60.135(c), but it has not been designed as a waste form.

At present, subcomponents of the waste forms are generally not allocated a function in meeting the NRC requirements for the EBS, except for the cladding in the case of spent fuel. Items such as the glass waste pour canister could be assigned a function, but current plans are to use as few components as possible to meet the regulatory requirement.

ASSESSMENT OF POST-CLOSURE PERFORMANCE

Assessment of post-closure performance of the waste package and EBS is based on allocating performance for various waste package components toward overall design objectives. The goal is to meet the 10 CFR 60.113 performance objectives for the EBS. Computer modeling will be used in conjunction with testing to assess whether the performance allocations are met or exceeded. *Because of the unprecedented time period* considered, computer modeling is essential. A significant issue will be validation of the computer models.

Distinctions must be made among models and codes. The assessment will be performed by an assessment code that will be integrating many conceptual models and process codes. For the Yucca Mountain waste package, the assessment code is PANDORA[3]. A conceptual model is a statement of assumed mechanisms that describe observed phenomena. An example would be a spent fuel release model. This conceptual model is evaluated by process codes which are detailed simulations of a physical or chemical process based on sound fundamental understanding of the

mechanism of the process. An example would be EQ3/6[4], a thermodynamic equilibrium geochemical code with kinetic capability.

A conceptual model may embody numerous mechanisms. For example, the spent fuel release model will need to include: cladding failure, fuel oxidation, gaseous release, dissolution from cladding and hardware, dissolution from gap-grain boundary inventory, dissolution from UO_2 matrix, and precipitation of secondary phases. These mechanisms are related and complex, and the integrated final release calculation must address all of them. Other models, such as that for container degradation, are equally complex, as they must address multiple mechanical and metallurgical degradation mechanisms.

The waste package performance assessment codes address three questions: (1) How much will each waste package's performance contribute to the performance of the ensemble of waste packages in the repository? (2) How will the ensemble performance compare to the NRC performance requirements and to the quantitative design objectives? (3) How much uncertainty is there in the predicted performance?

The current code, PANDORA1, is a deterministic code for a single package. The ensemble code will use PANDORA as a kernel, look at both deterministic and probabilistic variations among waste packages, and sum the results over all waste packages. [Examples of variable factors are: (a) container temperature as a function of contents and of location in the repository; (b) weld residual stress.] Uncertainty analysis will address both modeling and data uncertainties. The goals are to characterize uncertainties, identify those which may need further investigation, and ultimately reach a condition where remaining uncertainties are sufficiently bounded so as not to invalidate the resolution of the performance issues with reasonable assurance.

PANDORA is composed of seven coupled process modules. These are the radiation, thermal, mechanical, environmental (flow of water), corrosion, waste form alteration, and radionuclide transport modules. These process modules are summaries of the results of detailed process codes. There are numerous detailed process codes. An example is the familiar ORIGEN II[5], used to calculate the radionuclide inventory and other characteristics of the spent fuel. EQ3/6, a thermodynamic equilibrium and kinetic geochemical code, is used to calculate the results of rock-water, metal barrier-water, waste-water, and rock-water-metal-waste interactions. TACO[6] is used for the temperature field and TOUGH[7] for the fluid and heat flow in the repository near-field.

Several examples illustrate the relation between the detailed process codes and the assessment code. For thermal analyses, the detailed process code is TACO, a 2-D or 3-D transient heat transfer code. The thermal process module in PANDORA is a 1-D equilibrium heat transfer code that uses boundary conditions established by TACO or TOUGH or a similar detailed process code. The simple higher level calculations are validated against the detailed process code, and in this case bounded by the detailed code. Another type of relation is illustrated in cases where the geochemical code EQ3/6 is the detailed process code. Here the waste form alteration and radionuclide transport process modules in PANDORA use look-up tables generated by EQ3/6. These two methods, use of look-up tables or using the detailed process code to calibrate the system code, are those used to link the PANDORA process modules and the detailed process codes.

The distinction among assessment codes, detailed process codes, and conceptual models is significant with respect to code validation. The detailed process codes can be validated against many data sets, including geologic processes that extend for millions of years. Similarly, the conceptual models are amenable to direct verification with tests and experiments as well as natural analog data on geologic and archeologic time-scales. The simple process modules in the assessment code can also be validated by comparison with detailed process codes. While the difficulties of the above validations should not be underestimated, there are at least data sets against which the codes and models can be tested. By contrast, there seems to be no direct validation for the overall assessment code. It seems likely that the assessment code will be indirectly validated by methods such as peer review by an independent panel of experts. Such a validation will likely evaluate both the assessment code and the underlying conceptual models and detailed process codes.

In order to carry out an assessment with any of the codes, scenarios must be selected and a specific design evaluated. Given a design, it is further necessary to assign the specific function to be performed by a system element and then to set some performance goal for that element. In assessment of the Yucca Mountain repository system, that process is formal and called "performance allocation." It is not the purpose of this paper to provide details of that process, but rather to explain the general concept as it applies to the Yucca Mountain waste package. Details of both the overall concept and the quantitative performance measures applied to waste package components are given in the Consultation Draft of the Yucca Mountain Site Characterization Plan.

A listing of possible waste package elements and their potential functions for a Yucca Mountain repository is given in Table I. The possible elements range from the bare fuel or glass waste at the center of the package out to the rock adjacent to the emplacement borehole. Some components are assigned no function in the current conceptual design. This may be for either of two reasons. In the case of the glass pour canister or the rock surrounding the borehole, it is because there has been a decision not to allocate performance to that element. They exist and are still part of the waste package system and affect processes in that system, but for the purpose of assessment of compliance with the 10 CFR 60 Performance Objectives, no quantitative performance goal has been established. For example, this means that in using PANDORA to assess release rate control, the glass pour canister will not be allowed to retard water access to the waste once the container is breached.

The second reason a possible component may be assigned no function is that it is absent from the design being evaluated. Current examples are packing material or a solid filler in spent fuel containers. In these cases, evaluations have shown that negative aspects of those elements outweigh potential benefits. Being absent from the design, they do not affect processes in the system and do not have to be included in the assessment. Several elements, such as fuel cladding (or fuel treatment and regulatory strategies not shown in the table), appear as alternates and will be invoked in specific instances if assessment shows that the margin for meeting the performance objective is too small.

Another class of elements is illustrated by the borehole liner. It has a specific function and is allocated performance for one purpose, namely, the 60.111 requirement for retrievability. At present it has no

Table I. Performance Allocation includes selecting system elements and identifying functions for engineered barrier system at Yucca Mountain.

<u>Element</u>	<u>Function</u>	<u>Used at Yucca Mt.</u>
Bare fuel or glass waste	Provide very low dissolution rate in water	Yes
Fuel cladding	Prevent access of water to fuel	Yes
Glass pour canister	Prevent access of water to waste	No
Inert gas in container	Prevent oxidation of fuel during thermal peak	Yes
Solid filler in container	Change chemical environment near waste; prevent access of water to waste	No
Container	Prevent access of water to waste	Yes
Air gap between container and rock	Prevent water contact with container	Yes
Spacers between container and borehole edge or liner	Maintain air gap	Yes
Packing material	Does not serve saturated zone functions in unsaturated zone	No
Borehole liner	a) Maintain retrievability b) Control rock or water contact with container	Yes Possibly, no explicit plan
Engineered thermal field in repository	Thermal drying of adjacent rock to prevent access of water to container	Yes
Adjacent rock	Retard radionuclide release	No

post-closure performance allocation. However, it is available for the function of controlling rock or water contact with the container.

It is natural to question, "If a component exists in the system, why not claim credit for whatever function it could provide?" The answer is that "claiming credit" is not a simple process. It would be necessary to identify specific performance measures and set tentative goals, which would establish information needs, leading to a large set of tests, followed by assessments. The philosophy we have followed is to confine our assessments to the smallest and simplest set of components that will demonstrate "reasonable assurance" that the performance objectives are met. An example from among the selected elements illustrates this approach. The major EBS components for post-closure performance are the waste form and the container. All others have a supportive role. The preferred approach would be to show that the container alone will provide "substantially complete containment" and that the waste form alone will provide the $1 \text{ in } 10^5$ release rate control. Under conditions that are reasonable to expect at Yucca Mountain; i.e., less than a gallon of nonaggressive water per year per container, it may be possible to advance the argument that those elements alone would provide the required performance. It may, however, be difficult to demonstrate with "reasonable assurance" that such conditions are expected under "anticipated processes and events." For such a case, additional components can be invoked.

The simplest first step is to evaluate the two components acting together during each performance period. Should that approach be inadequate, additional elements can be invoked depending on the performance period to be addressed. For example, allocating performance

to the borehole liner will likely improve performance during the containment period, but may provide little assistance toward the end of the release control period.

A major purpose of performance allocation is to guide the testing program. If an element is not used in the design, obviously no testing program is required. For elements that exist but for which no performance is allocated, some testing is required to at least demonstrate that no deleterious effects are introduced. Alternate components need a rigorous evaluation program, though not as extensive as the components upon which primary reliance is placed. Ideally, one would carry out assessments prior to any testing. In practice at Yucca Mountain, this has been and continues to be difficult because the state of the art for codes dealing with flow and transport in an unsaturated fractured rock is well behind that for saturated flow and transport, and those under development suffer from a lack of in-situ testing data in unsaturated fractured rock to provide a basis for their validation.

For the waste package system at Yucca Mountain, most tests and experiments, either in the field or laboratory, are being designed and analyzed using detailed process codes. These detailed process codes have not yet been linked to the assessment code. The single package assessment code is in the process of achieving that link, but the ensemble and uncertainty codes lag behind. Our goal is to achieve a first integrated calculation to support Advanced Conceptual Design.

SUMMARY

The Engineered Barrier System, including the Waste Package, must meet two of the four post-closure performance objectives for the waste disposal system established by the NRC in 10 CFR 60. Both of these are for time periods of thousands of years. Therefore, computer modeling is required, and performance assessment is and will remain a key element of the waste package program through licensing.

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REFERENCES

1. United States Nuclear Regulatory Commission, Rules and Regulations, Title 10, Chapter 1, Code of Federal Regulations--Energy Part 60, Disposal of High Level Radioactive Wastes in Geologic Repositories.
2. Site Characterization Plan, Consultation Draft, DOE/RW-0160, January 1988.
3. O'Connell, W.J. and R.S. Drach, Waste Package Performance Assessment: Deterministic System Model Program Scope and Specification, UCRL-53761, Lawrence Livermore National Laboratory, Livermore CA, October 1986.
4. Wolery, T.J., et al., EQ3/6 Status and Application, UCRL-91884, Lawrence Livermore National Laboratory, Livermore CA, October 1984.
5. Croff, A.G., A User's Manual for the ORIGEN2 Computer Code, ORNL-TM-7175, Oak Ridge National Laboratory, Oak Ridge TN, 1980.
6. Burns, P.J., TACO2D - A Finite Element Heat Transfer Code, UCID-17980, Rev. 2, Lawrence Livermore National Laboratory, Livermore, CA, 1982.
7. Pruess, K. and J.S.Y. Wang, "TOUGH--A Numerical Model for Nonisothermal Unsaturated Flow to Study Waste Canister Heating Effects," Scientific Basis for Nuclear Waste Management VII, Materials Research Society Symposia Proceedings, Boston MA, November 1983, G.L. McVay (ed), Vol. 26, North-Holland, Elsevier Science Publishing Co., Inc., NY, pp. 1031-1038.