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Characterizing the Evolution of the In-Drift Environment in a Proposed Yucca Mountain Repository

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1. Introduction

This presentation provides a high-level summary of the approach taken to achieve a conceptual understanding of the chemical environments likely to exist in the proposed Yucca Mountain repository after the permanent closure of the facility. That conceptual understanding was then made quantitative through laboratory and modelling studies. This summary gives an overview of the in-drift chemical environment modelling that was needed to evaluate a Yucca Mountain repository: it describes the geological, hydrological, and geochemical aspects of the chemistry of water contacting engineered barriers and includes a summary of the technical basis that supports the integration of this information into the total system performance assessment.

In addition, it presents a description of some of the most important data and processes influencing the in-drift environment, and describes how data and parameter uncertainty are propagated through the modelling. Sources of data include

- external studies regarding climate changes
- site-specific studies of the structure of the mountain and the properties of its rock layers
- properties of dust in the mountain and investigations of the potential for deliquescence on that dust to create solutions above the boiling point of water
- obtaining thermal data from a comprehensive thermal test addressing coupled processes, and
- modeling the evolution of the in-drift environment at several scales.

Model validation is also briefly addressed.

2. Determining the processes to be quantified to evaluate the in-drift environment

Features, events and processes were identified iteratively in the process of coming to understand the potential range and evolution of in-drift environments, and are re-evaluated and updated as studies and experiments are designed and conducted and as modelling is done. The in-drift environment is addressed as part of a larger systematic approach to understanding the total system. Figure 1 illustrates the expected in-drift environment processes of incoming water and gas and dust, and their respective chemistries, as it relates to the features of the engineered system in a Yucca Mountain repository.

An important determinant of the in-drift environment is the amount and nature of seepage into emplacement drifts, over the long term, as well as initially during the period of above-boiling host rock temperatures. What needs to be known is the amount of seepage, its chemical characteristics including its colloid content, and its evolution in the drift environment. After there has been a breach of a waste package, additional chemistry changes and colloid formation at the waste form surface need to be addressed to allow the modelling of radionuclide transport away from the engineered system.

These thermal regimes are important to characterizing the in-drift environment over time. (Note that T_{wall} indicates temperature at the drift wall).

- Dry-out ($T_{\text{drift}} > 120^{\circ}\text{C}$, permanent closure in ~ 400 years) At the time of permanent closure the drift wall rock will be significantly dried out by years of forced ventilation, and emplacement drifts will be dry. After closure, temperatures in the emplacement drifts will increase for a few hundreds of years. Most repository drift wall temperatures will be greater than boiling (100°C), relative humidity will be low, and seepage of liquid water into drift openings will be unlikely. Waste package surface temperatures will be as much as 20°C higher than the nearby drift wall temperatures so the waste packages will also be very dry. Salts in dust on waste package surfaces may deliquesce. Deliquescence could promote localized corrosion.
- Transition ($120^{\circ}\text{C} > T_{\text{drift}} > 100^{\circ}\text{C}$, ~ 400 to $\sim 1,000$ years) When the drift wall cools locally below boiling (100°C), seepage of liquid water into the drifts will become possible, while the waste package surface temperature will still be high enough to permit the initiation of localized corrosion on contact with certain potentially aggressive water or brine compositions. Drip shields will prevent seepage from contacting the waste packages. The waste package and drip shield surface temperatures will be higher than the drift wall temperature, so seepage water will tend to evaporate if it contacts drip shields or waste packages, forming more concentrated solutions (e.g., brines). Based on predicted chemical characteristics of potential seepage from the host rock, these brines would be benign with respect to corrosion.
- Low Temperature Regime ($100^{\circ}\text{C} > T_{\text{drift}}$, $> \sim 1,000$ years) As the waste packages cool to a temperature below the threshold for crevice or localized corrosion in potentially deliquescent types of brines (at approximately 100°C , subject to uncertainty), waste package performance will be insensitive to the chemistry of any contacting water. At below-boiling temperatures the in-drift relative humidity will be higher, so evaporated solutions cannot be as concentrated, and will be benign.

From this description it is clear that temperature, relative humidity, seepage chemistry, the quantity of seepage that makes it onto a waste package, are items that need to be known in order to evaluate the system's behaviour. These conditions and process are illustrated in Figures 2 and 3. Note in Figure 2 the zone of vaporization that is a response to the heat emanating from the waste packages. The nature of the water that may eventually enter a drift as the repository cools is determined by taking into account the history of water in this dynamic system. In addition, a capillary barrier effect at the drift wall will always act to prevent or greatly reduce the amount of seepage entering the drift.

If water enters a drift, however, the major ion chemistry of contacting deliquescence products, evaporative brines, and seepage, need to be known within the context of the previously enumerated conditions. In addition, water will be moved around the drift as vapour during the period when there is still significant heat output from waste packages (Figure 3).

There is a small likelihood that salts in dust and left behind by evaporation will be of the purity and type to absorb water from air at the elevated temperatures needed to increase the potential for localized corrosion. It is an identified process and thus had to be evaluated. Although the occurrence of the hygroscopic part of this process is unlikely, it needed to be considered as a possible cause of waste package corrosion (Figure 4).

Eventually, on-package, and especially in-package, solution chemistry changes are expected as corrosion occurs and water enters waste packages. That changing chemistry, and also the resulting corrosion products will play a role in controlling eventual radioactive releases. These processes represent the opportunity to now roll all the previously illustrated processes into an evaluation of engineered system performance (Figure 5).

Features and processes need to be carefully identified and evaluated. Events that are likely, such as low-intensity earthquakes, are identified and evaluated and addressed in the design of the repository's engineered barriers. Events that are unlikely are also identified and evaluated, but are not discussed in this paper.

Figure 2. Schematic of processes determining water characteristics during the thermal period in rock above drifts in a Yucca Mountain repository

Figure 3. Schematic of near-drift and in-drift processes for nominal case

Figure 4. Schematic of processes controlling potential deliquescence on salts in dust accumulated on the metal barriers of a Yucca Mountain repository engineered system

Figure 5. Schematic of engineered system features and processes after thermal period

3. Data sources and model calibration

The modelling of features and processes relating to the behaviour of the engineered barrier system in a Yucca Mountain repository is based on a comprehensive site characterization program that included laboratory and field testing on several scales as well as the consideration of natural analogue information. Perhaps the most important single test conducted was a drift-scale heater test that heated rock for four years and is still in the process of being studied as it cools down now (via natural convection), also for four years. The battery of observations made and samples taken is too involved to recount in this paper. However, a layout of the test, illustrated in Figure 6, gives an indication of the comprehensiveness of this effort in terms of rock stability, hydrology, thermal, and chemical data taken.

Figure 6. Schematic of Yucca Mountain drift-scale heater test

4. Evaluating the modelling: confidence-building activities and validation

The modelling has been evaluated through internal and external reviews, and confidence has been built by applying models of drift-scale processes, especially temperature, moisture content and relative humidity, to predict test conditions prior to testing and comparing with test results. Validation is a word used in the Yucca Mountain Project with a very specific definition that is compatible with regulatory guidance as embodied into internal quality-assurance requirements. Validation in this context does not mean the matching of prediction with reality, which is not possible in the realm of repository system safety evaluations. That definition says that a model is valid if it can be shown to be adequate for the purpose to which it is being applied. This in effect means that a valid model has a technical basis suggesting it to be appropriate for its use; it is 'fit for purpose.' The broader and more comprehensive that technical basis, the more confidence may be had in the model's output.

5. Conclusions

This paper summarizes some of what was presented in the workshop, which gave more detail. For the purposes of the workshop report, however, this paper focussed on the identification of features and processes for the expected case. The challenges to a subsystem performance-evaluation will typically come by the suggesting of processes not considered or not adequately considered. This need for comprehensive identification and evaluation of

processes extends to the analysis for unlikely event conditions as well, of course, but this paper is focussing on the expected, or nominal, case.

Data and other scientific observations provide the basis for modelling, and modelling needs to be verified and reviewed to be credible. In addition, a series of steps can and ought to be taken to assure that there is a basis for having confidence in the modelling being appropriate, fit for the purpose at hand. Taking these steps is called "model validation" in the US program given regulatory guidance implemented into a quality-assurance process.

6. Acknowledgements

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