SCENARIO DEVELOPMENT FOR PERFORMANCE ASSESSMENT:--SOME QUESTIONS FOR THE NEAR-FIELD MODELERS^a

G. E. Barr
Sandia National Laboratories
YMP System Performance Assessment
Department 6312
Albuquerque, NM 87185
(505) 844-8532

R. W. Barnard
Sandia National Laboratories
YMP System Performance Assessment
Department 6312
Albuquerque, NM 87185
(505) 845-8403

SAND--92-2784C

DE93 008410

ABSTRACT

In an attempt to achieve completeness and consistency, the performance-assessment analyses developed by the Yucca Mountain Project are tied to scenarios described in event trees. Development of scenarios requires describing the constituent features, events, and processes in detail. Several features and processes occurring at the waste packages and the rock immediately surrounding the packages (i.e., the near field) have been identified: the effects of radiation on fluids in the near-field rock, the pathdependency of rock-water interactions, and the partitioning of contaminant transport between colloids and solutes. This paper discusses some questions regarding these processes that the near-field performance-assessment modelers will need to have answered to specify those portions of scenarios dealing with the near field.

INTRODUCTION

As the Yucca Mountain Project characterizes a potential site for a nuclear-waste repository, its performance-assessment effort is developing scenarios. The word "scenario" is used here to mean a well-defined sequence of features, events, and processes (FEPs) that ends with a release of radionuclides to the accessible environment. The sequence must consist of a logical and physically possible combination of FEPs—from an initiating feature, event, or process (such as groundwater flow, or an earthquake) to a final release. To construct scenarios we must synthesize the available information about the repository's natural setting, engineered components, and waste inventory. For

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government nor any agency thereof, nor any of theil Government. Neither the United States Government nor any agency thereof, nor any of theil employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, opposes disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The view and caninons of authors expressed herein do not necessarily state or reflect those of the

MASTER

de

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

^a This work was performed under the auspices of the U. S. Department of Energy, Office fo Civilian Radioactive Waste Management, Yucca Mountain Site Characterization Project, under contract DE-AC04-76DP00789.

organizing this large amount of information, we use "FEP diagrams," which may be described as generalized event trees. The eventual examination of compliance with regulations will rely on modeling of scenarios drawn from the FEP diagrams. The diagrams must therefore contain enough detail for the scenarios to express the complexities that lie behind the diagrams.

This paper will consider a component of the "nominal groundwater-flow" FEP diagram to investigate some of the details of the interactions between the nuclear waste, the engineered barrier system (EBS), and the repository rock surrounding the EBS. Previous analyses, such as PACE-90,1 or the 1991 Total-System Performance Assessment (TSPA) analysis,² did not consider near-field interactions in detail. (These analyses assumed a design of the potential repository based on the Yucca Mountain Site Characterization Plan (SCP);3 thin-walled waste packages emplaced vertically in boreholes with an approximatly 3-cm air gap.) We will focus on three issues that arise in part from recent work by others: the effects of the radiation field on fluids outside the waste package; the path dependency of rock-water interactions; and the partitioning of contaminants between solute and colloid mobilization and transport.⁶ As the interactions are developed here, specific questions and uncertainties in interpretations will become apparent. In order for the performanceassessment analysts to completely define the nominalflow scenarios, these detailed questions regarding near-field interactions must be resolved. This paper will pose the questions, for which other workers must provide some answers, to resolve the questions and uncertainties. FEP diagrams will be used to show different levels of detail as an aid to discussing the issues.

NOMINAL-FLOW FEP DIAGRAM

The nominal-flow FEP diagram describes the interaction of groundwater with the nuclear waste in the repository. The interactions can occur because of mechanical, thermal, chemical, and radiological effects that locally alter the waste containers and the surrounding rock (i.e., in the near field); as a consequence, the EBS might fail. There could then be transport of contaminants out of the emplaced waste into the surrounding rock of the near field. The presence of contaminants in the near-field rock could cause further alterations to the near field. Figure 1 shows a segment of the nominal-flow FEP diagram describing the interaction of flowing groundwater with the repository. This figure shows an overview of the processes; the main branches of this tree have been drawn to show the thermal effects groundwater interactions with either a "hot repository" or a "cold repository." In Figure 1, the groundwater-EBS interactions, which will be the focus of the rest of the discussion, are the contained in the FEPs "Actively Altered K, s" (hydraulic conductivity, K, and storativity, s), "Degradation of EBS," and "...Mobilization of Contaminants," this discussion will deal only with the "hot repository" branch. To provide more details concerning these FEPs, we must analyze the near-field and fluid-flow paths that are developed.

A. Alterations to the Near Field

Specifics of each of these FEPs rest on the physical characteristics of repository design. Figure 2 shows the waste-emplacement scheme in the SCP repository design.⁶ The important elements in this analysis are the repository drift, the drift backfill, and the waste container. Construction of the drift and emplacement hole introduces a free surface in the rock. This free surface alters the stress state and produces local strain to relieve the stress. Concentric and radial fractures are superimposed on the existing fracture sets, which might also be altered.

The waste container is inserted into the emplacement borehole with an air gap surrounding it. The waste has a coupled radiation and thermal history; for instance, the early thermal output could be dependent on γ -radiation emitters that produce heat and radiation outside the containers while the long-term thermal output could be dependent primarily on β and α emissions that are generally confined to the container. The thermal output of the containers, which are located in an unsaturated

medium, produces two-phase flow in the medium. Some of the possible consequences of that two-phase flow are shown in the three branches in the "hot-repository" section of Figure 1 (e.g., the "Condensation-Cap Flush" FFP in the leftmost branch of Figure 1).

The radiation field around the container extends out to tens of centimeters into the surrounding near-field rock. This radiation field consists largely of γ radiation, whose attenuation in the rock (and accompanying energy deposition) is illustrated in Figure 3. Table 1 lists the isotopes in LWR spent fuel that produce the greatest γ output after 10 years' decay. From the table, it can be seen that the e-folding distances (i.e., distance over which the intensity decreases by a factor of 1/e) range from about 2.7 cm for the 160-keV γ of ²⁴¹Pu to about 7.5 cm for the 1.6-MeV γ of ¹⁵⁴Eu. The distances into the rock for which 99% of the γ radiation is attenuated (about five e-folding distances) range from about 13 cm to 38 cm.

Table 1 γ-Radiation Characteristics of Major Isotopes in LWR Spent Fuel

(Based on 33,000 MWd/MTHM burnup of PWR fuel, 10-year decay)

Isotope	Inventory (Ci/MTHM)	Percent of 10-year Inventory	Half-life (years)	Typical γ energy (keV)	e-Folding Distance (cm)	Distance for ~99% attenuation (cm)
Cs-137	8.21E+04	21.0	30.2	661	4.7	23.6
Ba-137m	7.77E+04	19.9	3.80E-06	661	4.7	23.6
Pu-241	7.76E+04	19.9	13.2	160	2.7	13.5
Cs-134	5.22E+03	1.3	2.0	1400	7.3	36.3
Kr-85	4.85E+03	1.2	10.7	514	4.4	22.2
Eu-154	4.69E+03	1.2	16.0	1600	7 .5	37.7
Co-60	2.12E+03	0.5	5.3	1332	6.3	31.4

The longest half-life given in Table 1 is about 30 years. After about 1000 years, the γ -radiation field will therefore be essentially zero. Because previous analyses, such as PACE-90 and TSPA-91, assumed isothermal conditions in the repository, the radiation field is assumed to have decayed away and the thermal field is essentially steady-state.

B. Near-field interactions in a hot repository

Because of the presence of the emplacement hole (and drift), the rock is subjected to stress and strain changes. Heating produces compression and differential movement in and around the emplacement hole. Consequently, a well-connected set of fractures around the container should result. Flow of air and water vapor in a thermally driven convective flow field will occur through this altered zone, even if spall bridges the air gap. Because the flow is inside the radiation field, radiolytic production of H₂, HNO₃, and NH₄OH will occur in the air gap and in the nearby rock.⁴

The consequence of these effects is that aggressive vapors and fluids could circulate in the surrounding rock and interact with the waste package, driven by heat from the waste. The fluids could also interact with the rock, possibly altering the flow paths for circulation. The fractures, thermal gradients, and radiation fields might produce variable reaction paths in space and time,⁵ which in turn might produce different mineralizations at different locations. (The term "reaction path" is used in its broadest sense—inlcuding both the physical location of the reactions and the time-progression of the reactions). The mechanical, thermal, and radiation effects therefore couple the waste package, the fluids and vapors, and the rock in the near field.

As an illustration, one might expect silica dissolution and calcite precipitation to occur close to the container. Do these processes produce different permeability changes with and without the radiation field? As the waste container corrodes, when does enough iron appear in the immediately surrounding rock to influence precipitation from the flow stream? Will permeability changes direct more vapor flow to containers or more vapor flow between containers? The extent of dryout and volumetric limits on available water depend on knowing this. Do high temperature and the alteration of flow paths change the pH at the waste package? At Rainier Mesa, pore water is known to have a different composition from fracture water. The longer residence time in pores leaches sulfides from decomposing glass, which in the phreatic zone can oxidize to provide sulfuric acid.

As Figure 1 suggests, these effects could be substantially different if the repository is cold enough to produce no convective flow. The additional detailed FEPs developed here are shown in Figure 4, which shows a section of Figure 1 in more detail.

Now, instead of representing the near-field interactions simply as "Actively altered K, s" or "Degradation of EBS," the specific mechanisms are shown.

This discussion has pointed out some of the details that must be resolved to fully characterize the FEPs "Actively altered K, s" and "Degradation of EBS." Some of the uncertainties and questions are: What reactions control the near-field flow path and for how long do these changes persist? Additionally, what coupling occurs among these near-field interactions? For multiphase flow, how do radiolysis products alter the flow path? The FEP element, "...Mobilization of Contaminants," is intimately connected with the processes described above. In essence, what are the geochemical constraints with which performance assessment should be concerned?

C. Mobilization of contaminants

Release of contaminants requires some process for transfer of mass from the waste through the near field and on to the accessible environment. Currently most models of near-field mass transfer are for solutes in a virtually radiation-free field (e.g., see the comprehensive work by Pigford *et al.*⁷), implying times after emplacement when the radionuclide inventory is dominated by actinides. The models for solutes in high γ -radiation fields and for colloids under all circumstances are less well developed.

Waste-package failure, whether augmented by radiolysis or not, influences the local chemistry as the materials used in the container interact with the waste form and the external influences. One might expect, for example, that hydrolysis of iron in the container would affect how contaminants are partitioned between solutes and colloids. Further, flow paths could be modified by the inclusion of these materials in the reaction process. Such modifications could constrain the flow path and affect the distribution of contaminants around a breached container. These issues can be summarized for the scenario developers as: how contaminants are partitioned between solutes and colloids, how reaction paths are altered, and how alterations to reaction paths are different for solutes and colloids.

Summary

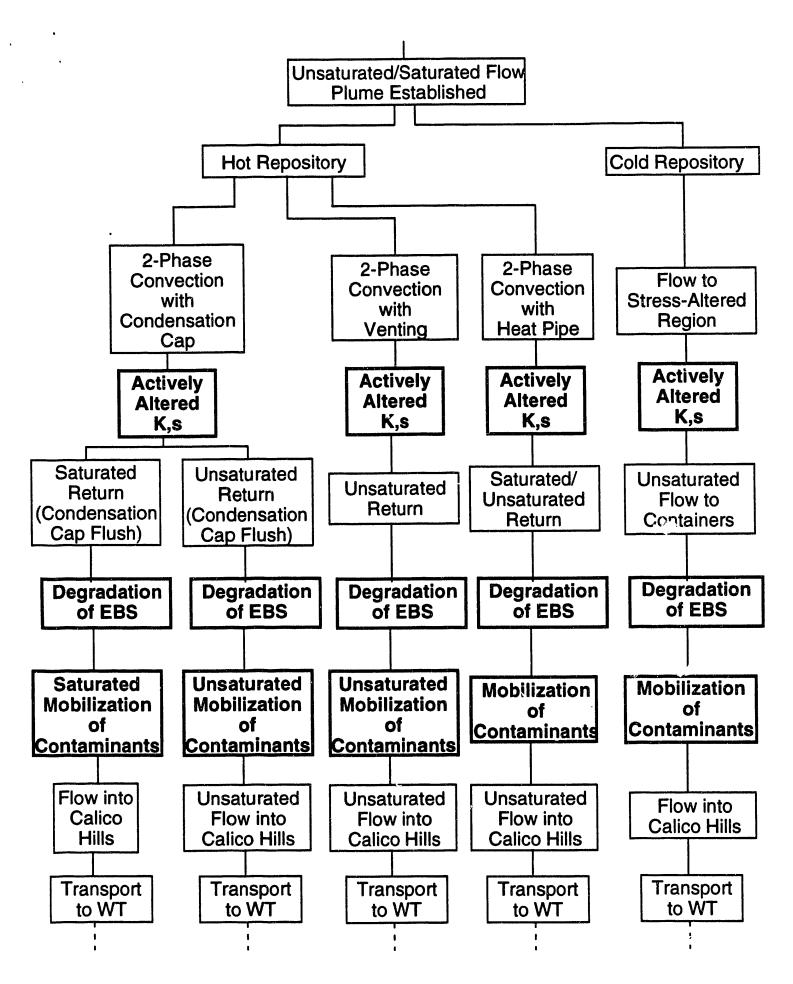
Future TSPA analyses for the potential Yucca Mountain repository will include thermal effects. From this discussion, it can be seen that both the thermal and radiation fields must be considered in order to include possibly important processes related to container failure and transport of waste. The FEPs described here are based on information and theories not currently included in the DOE-sponsored totalsystem performance assessments. As the scenarios are developed further, there will undoubtedly be revisions.

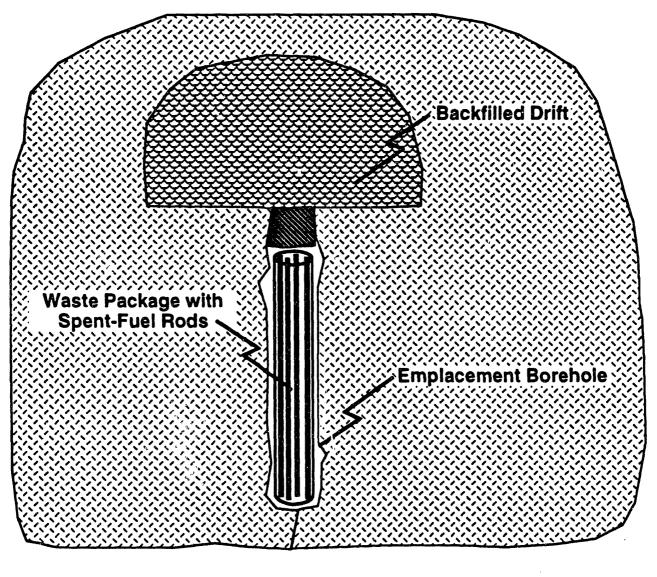
This analysis has introduced details to the nominal-flow FEP diagram that were not included in the overview diagrams (Figure 1). This additional level of detail will necessarily be part of the scenario definitions, and it is included in more detailed depictions of the nominal-flow event tree (Figure 4). At this stage, the additional details have not been resolved; indeed, more questions have been asked than have been answered. To get these answers, performance-assessment analysts and the specialists working on aspects of the EBS and near-field interactions must confer and collaborate.

References

- Barnard, R. W., and H. A. Dockery, editors., 1991, "Technical Summary of the Performance Assessment Calculational Exercises for 1990 (PACE-90), Vol. 1: 'Nominal Configuration' Hydrogeologic Parameters and Calculational Results," SAND90-2726, Sandia National Laboratories, Albuquerque, NM.
- Barnard, R. W., M. L. Wilson, H. A. Dockery, J. H. Gauthier, P. G. Kaplan, R. R. Eaton, F. W. Bingham, and T. H. Robey, 1992, "TSPA 1991: An Initial Total-System Performance Assessment for Yucca Mountain," SAND91-2795, Sandia National Laboratories, Albuquerque, NM.
- 3. Department of Energy (DOE), 1988, "Site Characterization Plan, Yucca Mountain Site, Nevada Research and Development Area, Nevada," DOE/RW-0199, U.S. Department of Energy, Washington, DC.
- 4. D. T. Reed and R. A. Van Konynenburg, 1991, "Effect of Ionizing Radiation on the Waste Package Environment," in *Proceedings of the Topical Meeting* on Nuclear Waste Packaging, Focus '91, American Nuclear Society, La Grange Park, IL, pp. 1396-??.
- 5. C. I. Steefel and A. C. Lasaga, 1992, "Putting Transport into Water-Rock Interaction Models," *Geology*, **20**, 1992, pp. 680-684.

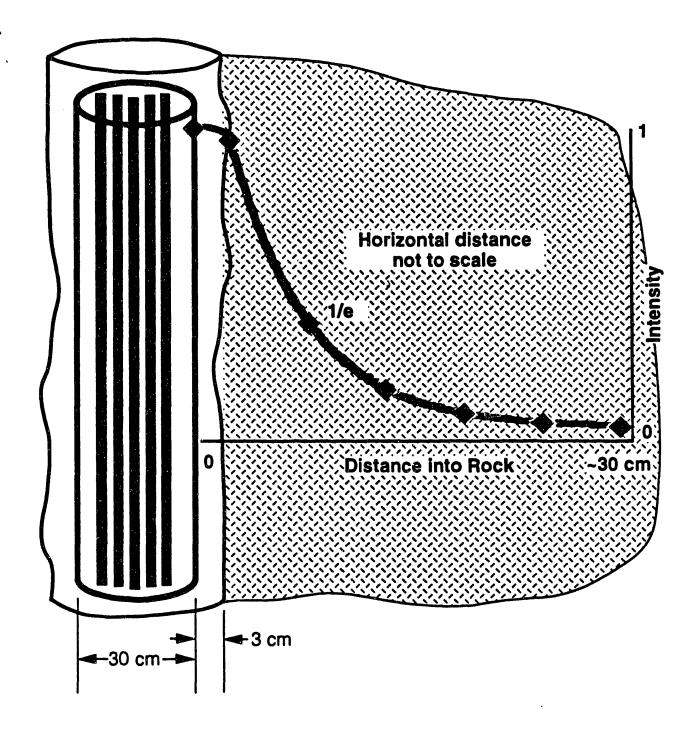
- 6. Bates, J. K., J. P. Bradley, A. Teetsov, C. R. Bradley, M. Buchholtz, 1992, "Colloid Formation During Waste Form Reaction: Implications for Nuclear Waste Disposal," *Science*, **256**, pp. 649-651.
- 7. T. H. Pigford, P. L. Chambré, and W. W.-L. Lee, 1992, "A Review of Near-Field Mass Transfer in Geologic Disposal Systems," Radioactive Waste Management and the Nuclear Fuel Cycle, 16(3+4), 1992, pp. 175-276.





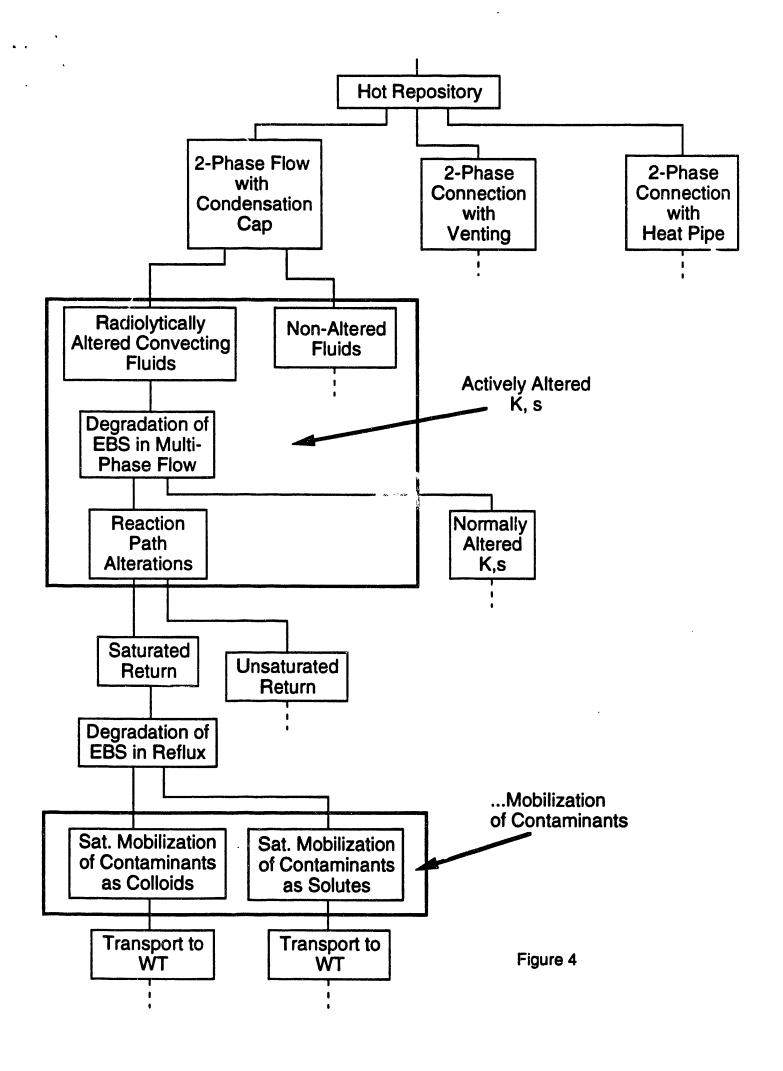
(not to scale)

Figure 2



Gamma intensity as a function of distance from waste package

Figure 3



DATE FILMED 5/13/93

			•	
-				