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Subject: Transmittal of "Effects of Design on Coupled Thermal-Hydrologic-Chemical Effects on Seepage and Flow—Letter Report" (IM 1402.561.020)

Dear Dr. Leslie:

This letter transmits Intermediate Milestone "Effects of Design on Coupled Thermal-Hydrologic-Chemical Effects on Seepage and Flow—Letter Report" (IM 1402.561.020).

This report was prepared under the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (KTI) following guidance received on January 10, 2000, February 9, 2000, and April 18, 2000, and based on discussions held with you by telephone and during your visits to CNWRA. The content of this report represents an approach to updating the ENFE Issue Resolution Status Report (IRSR) with regard to the subissue on Effects of Coupled Thermal-Hydrologic-Chemical Processes on Seepage and Flow. The intent of the update is to reflect reviews of U.S. Department of Energy (DOE) process model reports (PMRs) and analysis models reports (AMRs) using the acceptance criteria and review methods from the Yucca Mountain Review Plan (YMRP), Revision 0. The starting point for this letter report was Sections 4.1 and 5.4 of Revision 2 of the ENFE IRSR. As directed, only minor modifications have been made to Section 4.1 from Revision 2 of the ENFE IRSR to reflect design changes proposed since the DOE Viability Assessment (VA). Section 5.4 has been substantially rewritten and reorganized to focus on features, events, and processes (FEPs) and the DOE models, abstractions, and analyses.

Most of the AMRs and the relevant PMRs are not available for review as of this writing. The resolution status in this document is based on information contained in the License Application Design Selection Report, Revision 3 of the Repository Safety Strategy, the TSPA-SR Methods and Assumptions Report, the Unsaturated Zone Flow and Transport PMR, and the AMR on Drift Seepage Model for Performance Assessment. It is anticipated that the resolution status of this subissue will be updated further as the more detailed AMRs and PMRs become available for review. In addition, during DOE quality assurance audits, information may become available which will be incorporated as appropriate.

This document shows one method of organizing the IRSR to reflect the current NRC licensing approach. The method used here differs somewhat from that used in the first three deliverables in this series consistent with the most recent NRC instructions. We are now using these four deliverables to develop the ENFE IRSR. We understand that the IRSR text will likely change as DOE design continues to evolve, AMRs and PMRs become available for review, and the YMRP is modified for Revision 1. This report documents our continued attempts to reorganize an IRSR to reflect the YMRP structure, and will result in a more direct relationship between the YMRP and the technical bases used to prepare the Safety Evaluation Report than is currently available. Specific sections of the YMRP addressed by this deliverable include spatial and temporal distribution of flow, quantity and chemistry of water contacting the waste, and advective flow paths in the unsaturated zone.

If you have any questions about this deliverable, please call me (210-522-5540) or Dr. Roberto T. Pabalan (210-522-5304).

Sincerely yours,

English C. Pearcy
Geohydrology and Geochemistry Manager

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1.0 INTRODUCTION

The U.S. Department of Energy (DOE) has committed to prepare a series of Process Model Reports (PMRs) and supporting Analysis Model Reports (AMRs) as the technical bases for the Total System Performance Assessment (TSPA) for the Site Recommendation (SR). The purpose of this letter report is to update the resolution status of the subissue on the effects of coupled thermal-hydrologic-chemical (THC) processes on drift seepage and flow in the unsaturated zone (UZ) based on a review of the information presented in the PMRs and AMRs. This update is intended to support Revision 3 of the Issue Resolution Status Report (IRSR) of the Evolution of the Near-Field Environment (ENFE) Key Technical Issue (KTI). The following reports are a subset of those that have been identified in the DOE AMRs/PMRs schedule as being relevant to the ENFE subissue on seepage and flow: PMR on UZ Flow and Transport, U0075–AMR on Seepage Model for Performance Assessment (PA), N0120–AMR on Drift Scale Coupled Processes, U0120–AMR on Drift Seepage Including Coupled Processes, U0105–AMR on Mountain Scale Coupled Processes, and N0080– Features, Events, and Processes (FEPs) for the Near-Field Environment.

Of the relevant AMRs and PMRs, only U0075 (CRWMS M&O, 2000b) and PMR-UZ (CRWMS M&O, 2000c) are available for review as of this writing. In the following sections, the resolution status is based on these two documents and the license application design selection (LADS) report (CRWMS M&O, 1999a), the TSPA-SR Methods and Assumptions Report (CRWMS M&O, 1999b), and the Revision 3 of the Repository Safety Strategy (CRWMS M&O, 2000a). It is important to note that the TSPA-SR Methods and Assumption Report does not contain details on how the different modeling approaches will be implemented. The resolution status of this subissue will be further updated as more AMRs and PMRs become available for review.

4.1 THE EFFECTS OF COUPLED THERMAL-HYDROLOGIC-CHEMICAL PROCESSES ON SEEPAGE AND FLOW

In Revision 3 of the Repository Safety Strategy (CRWMS M&O, 2000a), the DOE identified seven principal factors of the postclosure safety case. Three of these principal factors are potentially affected by persistent THC alterations of the flow properties: limited seepage of water into the emplacement drifts, retardation of radionuclide migration in the UZ, and dilution of radionuclide concentrations during migration. Secondary factors identified by the DOE for the postclosure safety case, though given lower importance, include Coupled Processes—Effects on UZ Flow, Coupled Processes—Effects on Seepage, and Advective Transport in the UZ.

The model abstraction section of the Yucca Mountain Review Plan (YMRP) (U.S. Nuclear Regulatory Commission, 2000a) is broken into 14 different abstractions. These abstractions are equivalent to the integrated subissues (ISI) in theTotal System Performance Assessment and Integration IRSR (U.S. Nuclear Regulatory Commission, 2000b). Three of the ISIs are relevant to ENFE Subissue 1: spatial and temporal distribution of flow, quantity and chemistry of water contacting the waste, and advective flow paths in the UZ.

Drift seepage enters into a PA framework through the Nuclear Regulatory Commission (NRC) ISI on spatial and temporal distribution of flow and the ISI on quantity and chemistry of water on the waste package. Drift seepage depends on flow properties at the tunnel crown, and is thus potentially affected by THC-induced changes in these properties. Radionuclide dilution enters into a PA framework through several ISIs. One of these ISIs—advective flowpaths in the UZ—is potentially affected by THC-induced changes. In particular, dilution in the UZ depends on the advective flowpaths through this zone and on the distribution of flow between matrix and fractures, which are potentially altered by THC processes. The principal factor retardation of radionuclide migration is also covered by several ISIs, one of which is relevant to this subissue: flow paths in the UZ. THC-induced changes in flow paths can affect retardation indirectly by altering the fraction of contaminants passing through highly sorbing zones. For example, THC-induced changes in rock flow properties may alter the partitioning between the fractures and the more sorbing matrix or cause highly sorbing zeolitic zones to be bypassed.

Contributions from the Unsaturated and Saturated Flow Under Isothermal Conditions (USFIC) KTI (U.S. Nuclear Regulatory Commission, 1999a) and the Thermal Effects on Flow KTI (U.S. Nuclear Regulatory Commission, 1999b) will be required, in addition to those of the ENFE KTI, to successfully address the concern of THC effects on seepage and flow. DOE must adequately address the potential for coupled THC processes to alter seepage and flow in its assessments of repository performance.

4.1.1 Review Methods and Acceptance Criteria

The DOE approach to evaluate and abstract coupled THC processes affecting seepage and flow in a TSPA for the proposed repository at Yucca Mountain (YM) is satisfactory if specific acceptance criteria are met. With this revision (Revision 3) and update of the ENFE IRSR, the acceptance criteria and review methods that will be used to evaluate the DOE approach have been moved to the appropriate ISI sections of the YMRP, Revision 0.

4.1.2 Technical Bases for Review Methods and Acceptance Criteria for Effects of Coupled Thermal-Hydrologic-Chemical Processes on Seepage and Flow

The technical bases are primarily focused on explaining why the results of THC coupled processes may be important to seepage and flow. Past PA analyses of the effects of coupled THC processes on the potential repository seepage behavior and groundwater flow have been limited. In addition, the relevance to performance of a particular coupled THC process is highly dependent on repository design (e.g., thermal loading strategy and materials used). This has resulted in acceptance criteria that primarily focus on ensuring that analysis of the effects is completed. The sophistication of the analysis of the effects of coupled THC processes on seepage and flow that could be found acceptable by staff depends on the significance to repository performance. The status of issue resolution is determined by the information available at the present, any plans to obtain the additional information as part of the long-term testing program, and the ability of codes to model coupled processes and determine their impact on repository performance.

For instance, results of coupled THC modeling (see Chapter 4 of Sagar, 1996, for an example) might be used to infer the potential amounts of primary minerals that are either dissolved or the mass of secondary minerals that may precipitate because the coupling. This information might be combined with existing site distribution of primary and secondary minerals (abundance, location in the matrix or fracture, or both) and the molar volume of the minerals to calculate the increase or decrease in porosity caused by the coupled THC process. If the resulting changes in porosity and other hydrologic properties are within the range of values sampled for a particular modeled hydrologic unit in the basecase PA, then the effect of coupled process on seepage and flow need not be considered further.

4.1.2.1 Coupled Thermal-Hydrologic-Chemical Processes Affecting Flow of Water

At YM, host rocks are silicic tuffs [70–80 percent SiO_2 (Byers, 1985)]. These rocks are variably vitric (glassy), devitrified, or altered. Devitrification of the glass results in an assemblage of silica minerals and alkali feldspar. The tuffs can be altered, primarily to the silica-rich zeolites, clinoptilolite, and mordenite, or to analcime at depth (Broxton, Bish, and Warren, 1987; Bish and Chipera, 1989). The saturated zone (SZ) groundwater is predominantly a dilute, oxidizing, sodium bicarbonate solution rich in dissolved silica. There is evidence from one well (UE-25 WT #17) that redox conditions can locally be mildly reducing (-100 mV $\leq$ Eh < 0 mV). The UZ groundwater differs substantially from SZ water, being more concentrated and dominated by calcium chloride or calcium sulfate in rocks nearer the ground surface (Yang, 1992; Yang, Peters, and Thorstenson, 1993; Yang, Rattray, and Yu, 1996; Yang, et al., 1996). Aqueous silica concentrations in excess of cristobalite saturation are observed in tuffaceous aquifers at YM (Kerrisk, 1987), and higher concentrations are observed in the UZ (Yang, et al., 1996). The high silica contents are generated by a reaction of infiltrating meteoric water with siliceous volcanic glass (White, Claassen, and Benson, 1980). Glass alteration in the Calico Hills formation below the repository horizon is accompanied by incongruent precipitation of mordenite and clinoptilolite. These minerals are zeolites with important sorptive characteristics (Ames, 1964; Pabalan, et al., 1998; Bertetti, Pabalan, and Almendarez, 1998). In the proposed repository horizon and the near-field environment at YM, the tuffs are devitrified to alkali feldspars and silica mineral polymorphs (cristobalite, quartz, and tridymite). Here, smectite is the dominant aluminosilicate alteration phase, occurring in abundances up to 5 percent (Bish, 1988). In lower volcanic units at YM, primary glass has been altered to analcime ± kaolinite rather than clinoptilolite. This mineralogic change, which is generally associated with the disappearance of cristobalite with depth, is consistent with a decrease in the activity of aqueous silica (Kerrisk, 1983). Fracture and cavity mineralogy is characterized by calcite, smectite, silica minerals, zeolites, and manganese oxides (Carlos, 1989; Carlos, Bish, and Chipera, 1991; Paces, et al., 1996).

The gas phase in the vadose zone at YM is primarily air, approximately saturated with water vapor and enriched in CO_2 relative to the atmosphere. Gas chemistry analyses show limited variability in the CO_2 content in space and time (Thorstenson, et al., 1990). The partial pressure of CO_2 in the gas phase has a strong effect on the pH of the coexisting groundwater, which, in turn, affects aqueous speciation, solubilities, and mineral stabilities (Arthur and Murphy, 1989; Murphy, 1993).

During elevated temperatures, the rates of alkali feldspar dissolution and growth of secondary phases, such as smectite, clinoptilolite, silica minerals, and calcite, would be accelerated. Thermodynamic analyses for smectites (Ransom and Helgeson, 1994) and clinoptilolites (Bowers and Burns, 1990) have quantified their decreasing stability with increasing temperature and decreasing aqueous silica content. In addition, the swelling capacity of uncompacted smectite has been shown irreversibly decreased by alteration in a water vapor environment at temperatures above 150 °C (Couture, 1985). Field evidence for temperature-induced changes can be obtained by regarding the natural environment at depth as an analog of the near-field environment (Apted, 1990). Observations at YM include the transitions with increasing depth from clinoptilolite to analcime to albite and from smectite to ordered illite/smectite to illite. The clay mineral data have been interpreted to give thermal profiles with temperatures ranging up to 300 °C for an extinct hydrothermal system at depth at the north end of YM (Bish, 1988; Bish and Aronson, 1993). Reduction in permeability of tuff adjacent to fractures has been documented in rocks near the intrusion of a basaltic sill (Matyskiela, 1997).

Experimental studies of the hydrothermal reaction of tuffs and natural waters from YM at 90 to 250 °C have been conducted (Knauss, et al., 1984; Knauss, Beiriger, and Peifer, 1987; Knauss, 1987). These studies demonstrate dissolution of primary minerals, precipitation of secondary phases, and variations in water chemistry. Secondary precipitation of clay minerals, zeolites, cristobalite, and calcite were observed. Experiments in which CO_2 loss occurred showed more extensive secondary mineralization and particularly more calcite precipitation than in pressurized closed-system experiments. Water chemistry variations were generally small and achieved approximately steady-state conditions in long-term experiments. The aqueous silica concentration was observed to increase substantially at elevated temperatures corresponding to the increased solubility of silica minerals. The water chemistry in selected experiments was reasonably represented as a function of time with partial equilibrium and kinetic reaction path models of the water-rock interactions (Delany, 1985). Application of the results of these experiments to the near-field environment at YM must be judicious, because the high temperatures, high pressures, saturated conditions, and short time scales of the experiments are unrepresentative of expected conditions at YM.

Mass transfer calculations that account for partial equilibrium and reaction kinetics in gas-water-rock interactions have provided geochemical models related to the YM site and near-field environment (Kerrisk, 1983; Ogard and Kerrisk, 1984; Delany, 1985; Arthur and Murphy, 1989; Murphy, 1993; Murphy and Pabalan, 1994; Lichtner and Seth, 1996). The aqueous silica concentration and the CO_2 pressure have been shown particularly important in defining the solid-phase assemblage and the aqueous-solution composition. At present, these models are limited principally by the lack of thermodynamic and kinetic data. However, there have been several recent attempts to obtain such data by experimental and estimation techniques (e.g., Bowers and Burns, 1990; Johnson, et al., 1991; Ransom and Helgeson, 1994; Murphy, et al., 1996, Chipera and Bish, 1997) which, in some cases, appear to yield inconsistent results. Calculations of time-dependent processes are further hampered by the difficulty in realistically characterizing reactive surfaces in geologic environments.

Coupled THC effects on seepage and flow may be affected by changes in porosity and permeability of the host rock. The porosity and permeability may be enhanced by dissolution of primary minerals that make up the matrix of the medium. Conversely, precipitation of secondary minerals may serve to plug available porosity, reducing permeability. Mineral solubilities depend on the pressure and temperature of the system of interest, as well as solution pH, $p(CO_2)$, $p(O_2)$, and salinity. Many common minerals, such as quartz and metal sulfides, exhibit a prograde solubility, whereby precipitation is favored with decreasing temperature. Silica scale in geothermal wells is due, in large part, to the cooling of fluids that are supersaturated, with respect to silica, as they rise to the surface (Thomas and Gudmundsson, 1989). In contrast, carbonates, such as calcite and dolomite, exhibit retrograde solubility and precipitate from solution with increasing temperature. Precipitation and dissolution also may be controlled by kinetic processes. For example, although calcite precipitates readily in geothermal systems, quartz precipitation is kinetically controlled at temperatures below 200 °C and may not occur under supersaturated conditions (Thomas and Gudmundsson, 1989).

Gas flow from the near field, driven by vaporization of water, is predicted to be away from the near field in all directions (Pruess, Wang, and Tsang, 1990; Tsang and Pruess, 1987). This process would tend to purge air containing O_2 from the near-field environment. The vapor pressure of water at temperatures above 95 °C exceeds the hydrostatic pressure of less than 0.1 MPa at YM. Thus, the gas phase in the near field would tend to be dominated by H_2O. The different minerals have different temperature-dependent solubilities. As a result, solutions (both liquid and gas) moving by thermally driven convection will redistribute chemical components such as pH, chloride, oxygen, CO_2, silica, and calcium.

Silica redistribution in the YM near-field environment is likely controlled by the dissolution of glass, feldspar, and cristobalite, and amorphous silica precipitation. The rate of this redistribution will depend on the aqueous silica activity and the relative rates of reaction. Silica redistribution has been observed in laboratory heater experiments with YM tuff under unsaturated conditions (Rimstidt, Newcomb, and Shettel, 1989). Silica and Fe, dissolved near the heater, were transported in solution and precipitated as amorphous silica, Fe hydroxides, clay, and zeolite at the cooled end of the system. In the nonisothermal, transient experiments of Lin and Daily (1990) on samples of the Topopah Spring Tuff, permeability was progressively reduced by three orders of magnitude from 1.3×10^{-14} m^2 to about 10^{-17} m^2 due to narrowing of fracture apertures by silica deposition. Experiments of Vaughan (1987) using granite cores indicated that, although porosity was reduced by a relatively small amount, permeability was reduced by more than 95 percent. Chigira and Watanabe (1994) also observed narrowing of pore throats by silica precipitation in flow experiments using powdered granite and amorphous silica powder. They calculated that at 90 °C porosity would be halved in 135 yr.

Bish (1993) developed a premise that the thermal regime will induce a progressive Ostwald ripening effect in which a sequence of zeolites will form and, if enough time is available, culminate in the most stable assemblage of albite and quartz. This alteration will lead to a net volume reduction, potentially increasing porosity and permeability.

The effects of chemistry on flow are commonly neglected in thermal-hydrologic (TH) simulations. For the viability assessment (VA) repository design and thermal loading pattern, development of an extensive region of countercirculating water and vapor above the emplacement drifts was predicted to cause changes in porosity, permeability, and solution composition during regulatory time frames of thousands of years (e.g., Hardin, 1998). Small changes in porosity can effect orders of magnitude changes in permeability (Lichtner and Walton, 1994). Thus, the dissolution and transport of silica, followed by precipitation during evaporation, could modify the permeability distribution around the repository horizon. Some numerical simulations have been performed in an attempt to predict the redistribution of pH, chloride, silica, and calcium in the near-field environment and the effect on permeability (Lichtner and Seth, 1996; Lichtner and

Turner, 1997). The increased drift spacing and lower areal heat loading in the Enhanced Design Alternative II (EDA-II) repository design may allow water to drain through the inter-drift regions and may prevent formation of a zone of perched condensate and the associated region of counter-circulating water and vapor above the repository. This potential lack of a vigorous heat pipe and refluxing decreases the likelihood of large changes in porosity and permeability above emplacement drifts.

Major geochemical changes in the near field are likely to depend primarily on the availability of water. Although unsaturated, the rocks at YM contain abundant water, commonly 10 percent of the rock volume. A large amount of zeolitic water is also available in certain horizons that could be released at elevated temperatures. Most extensive and rapid chemical reactions will occur where water evaporates, depositing solutes, and where water vapor condenses. Evaporation and mineral precipitation may occur in the rock matrix or in the fractures, depending on the local hydrologic conditions. Gaseous transport of water vapor to cooler zones of condensation, however, is likely to occur dominantly in fractures. Therefore, condensation of initially dilute acidic water, due to dissolution of gaseous CO_2 into the condensate, and mineral dissolution are likely to occur on fracture surfaces. Together, these processes could lead to changes in average permeability and in permeability distributions for matrix and fractures. If, however, water condensed on fracture surfaces dissolves minerals there and precipitates secondary phases with larger volumes before the water is imbibed, then fracture permeability could decrease as well. The locus of dissolution and precipitation reactions, with respect to fractures and matrix, could affect the hydrologic behavior of the near-field system, including seepage into drifts, and is presently poorly constrained in coupled hydrologic-chemical modeling.

4.1.2.2 Effects of Engineered Materials on Seepage and Flow

In the TSPA-VA design, the use of cementitious materials, in the form of concrete inverts and linings, was considered for the estimated 179 km of emplacement drifts of the proposed YM high-level waste (HLW) repository, in addition to the planned use of cement in roadways for construction, emplacement ramps, and service mains. In the EDA-II design, cementitious materials are not planned for ground support, except in the form of grout to anchor the rock bolts of the ground support system. The potential effect of cementitious materials on seepage and flow in the EDA-II design is expected to be substantially reduced compared to the TSPA-VA design. The current design, however, does call for large amounts of cementitious materials in ventilation shafts and in ventilation tunnels below the emplacement drifts.

Interaction of cement with the tuffaceous host rock and ambient groundwater could have an important effect on seepage. The chemistry of pore fluids in contact with hydrated cement phases is characterized by persistent alkaline pH (>10). Hyperalkaline cement pore water is thermodynamically incompatible with silica, a major component of the proposed YM repository host rock unit. Thus, migration of the high-pH cement pore water into the host rock is likely to result in strong alteration of the tuff. The Maqarin natural analog site for studying cement interaction in northern Jordan suggests that rapid interaction between cement-equilibrated pore waters and silicate-bearing rocks can be expected (Cowan, 1975). This may result in sealing of fractures and alterating of the host rock minerals. Calculations by Lichtner, Pabalan, and Steefel (1997, 1998) suggest that strong alteration of the tuff host rock at YM and of cement in contact with the tuff could result from interaction of cement and tuff pore waters and the respective minerals.

Because of the low silica concentration of the cement pore water, the host rock would begin to dissolve on contact with the hyperalkaline fluid (Lichtner and Eikenberg, 1995). Dissolution of tuff could lead to widening of the fractures and enhancement of seepage and groundwater flow through the repository. As the host rock dissolved and the silica concentration increased, calcium silicate hydrate (CSH) phases would precipitate and clog the pore spaces. Alternatively, precipitation of calcite and CSH phases along the interface of the fracture and matrix could seal the fractures from the matrix, producing isolated channels through which groundwater could flow. If sufficient amounts of calcite and CSH phases are precipitated along fracture walls,however, reduction in fracture porosity and permeability, or fracture plugging, could result in changes in seepage and groundwater flow through the repository. Reduction in horizontal permeability that might result from fracture plugging tends to increase seepage by limiting the capillary diversion effect, whereas the associated increase in capillary pressures tends to have the opposite effect. Results of Lichtner, Pabalan, and Steefel (1997, 1998) show that porosity reduction within the tuff matrix could isolate it from fracture pore water and could affect seepage. Precipitation of calcite would also occur, as the low CO_2-high Ca cement pore fluid mixes with the ambient groundwater containing high CO_2 concentrations (Lichtner and Eikenberg, 1995; Steefel and Lichtner, 1994).

The results of Lichtner, Pabalan, and Steefel (1998) indicate that calcification of the cement could occur as would be expected under ambient conditions. In counter-diffusive transport, calcification is more pronounced in a partially saturated system compared to a fully saturated one. Both the large block and drift-scale thermal tests could provide important insights that could constrain the potential effects on seepage resulting from cementitious materials interacting with the tuff.

4.1.2.3 Microbial Effects on Seepage and Flow

Within the last decade, data have been collected showing the existence of diverse communities of microorganisms living in the deep subsurface environment (Amy and Haldeman, 1997). The role of microorganisms in many important geochemical phenomena long has been recognized (Ehrlich, 1996). Subsurface bacteria may mediate many processes that may impact a potential repository's performance. These processes include canister corrosion and leaching of the glass waste form. Other potentially important microbial processes are supplying organic byproducts as potential complexants and direct uptake of radionuclides and either immobilization or mobilization depending on whether the microorganism is attached to an immobile surface. Finally, microbial processes can alter pore-water and gas chemistry, and microbes can produce exopolymeric materials that may block pores and fractures in the rock matrix impeding the flow of water. Only the latter two processes are discussed in this subissue. The conditions necessary for microbial activity in relation to all these deep subsurface processes will be substantially the same and will be discussed next.

The potential importance of microbial processes to nuclear waste repositories has been recognized for more than 10 yr in international radioactive waste disposal programs (West, 1995). Extensive research and modeling programs are ongoing in other countries (Christofi and

Philp, 1997), particularly in Switzerland (Brown and Sherrif, 1998), Canada (Stroes-Gascoyne, 1996), the United Kingdom (West, 1995), and Sweden (Pedersen, 1996; Pedersen and Karlsson, 1995). While more work has been focused on low-level and intermediate-level waste repositories, because the quantity of organic carbon is greater than that expected for HLW repositories, several countries have assessed the potential importance of microbial processes in proposed HLW repositories (Christofi and Philp, 1997).

In contrast, microbiological study in the United States HLW program has not progressed as far in determining the importance of microbial processes to repository performance. The US efforts have focused on identifying microbial processes relevant to the YM site, determining parameters critical to evaluation of the disturbed environment (temperature and nutrients added), and identifying the most effective means to evaluate these two factors (Horn and Meike, 1995; Wilder, 1996). Microbes could compromise the integrity of a waste package (WP), modify water and gas chemistry outside the bounds predicted by abiotic chemical calculations, and alter the rate of radionuclide transport from breached waste packages WPs (Horn and Meike, 1995). Research efforts on the effect of microorganisms on radionuclide transport at YM were summarized and evaluated (Hersman, 1996). One conclusion from the Hersman study was that the elevated subsurface concentrations of CO_2, relative to the atmospheric concentration, ares the result of biogenic activity. Finally, an initial attempt to model the potential effects on repository performance of microbial processes in the near field has been proposed as part of the TSPA-VA (TRW Environmental Safety Systems, Inc., 1997). This effort will address potential changes in gas chemistry (CO_2) from microbial processes. The effort will rely on models developed in Europe to assess the potential importance of microbial processes on HLW repositories (TRW Environmental Safety Systems, Inc., 1997; Grogan and McKinley, 1990).

Horn and Meike (1995) reviewed the conditions necessary for microbial activity in relation to deep subsurface repositories, such as YM. For metabolic activity, microorganisms require an energy source (usually organic C); water; a source of N, S, and P; and suitable environmental conditions, such as temperature and pH (Horn and Meike, 1995). Most microorganisms are heterotrophic, using organic C compounds as their energy source. Oligotrophic bacteria (those that can grow in nutrient-poor water) require a minimum organic C content 1–15 mg L^{-1} of water (Ehrlich, 1996). The organic C content of the groundwater in the vicinity of the repository (J-13 well water) is in the range of 0.15–0.55 mg L^{-1}, composed principally of humic acids and low molecular weight fatty acids (Means, Maest, and Crear, 1983). This composition is well below the level suggested for oligotrophic bacterial growth. Nevertheless, microbial activity in the soil zone of the UZ is attributed as the reason for elevated CO_2 concentration in the gas phase (Hersman, 1996; Thorstenson, et al., 1998).

Unlike other international programs for HLW disposal where potential disposal sites are located in the SZ, the US site is located in the oxidizing UZ, which has a profound consequence on the potential importance of microbial processes at YM. The activity of microbes is limited in the UZ by the low water potential (Kieft, et al., 1993, 1997). Other limits on the potential for microbial activity in the subsurface of a waste repository include the available nutrients (N and P) and the increased temperature from radioactive decay (Pedersen, Motamedi, and Karnland, 1995).

Using samples collected from the exploratory studies facility (ESF), Kieft, et al., (1997) conclusively demonstrated that water is the major limiting factor to growth and microbial activity at YM. Microbial abundance was low. Indicated microbes were generally most abundant in locations from less consolidated, nonwelded, or bedded tuffs, such as the Paintbrush Tuff (Kieft, et al., 1997). The additions of N and P to crushed tuff samples resulted in little further simulation of microbial activity. Addition of organic carbon to the crushed tuff samples stimulated growth more than just added water. Thus, there is a potential for increased microbial activity at YM with the addition of water and carbon.

The predominant mode of growth of bacteria in nature is as a biofilm attached to a surface, particularly in oligotrophic environments (Amy and Haldeman, 1997). Bacteria attach to solid surfaces where nutrients concentrate. These surfaces provide a more abundant food source than the bulk fluid. For saturated conditions, provided sufficient nutrients and carbon are present, the growth of microbes in biofilms and the production of exopolymeric materials by microbes can be sufficient to substantially reduce the permeability of rock units and soil (Amy and Haldeman, 1997).

The tuff at YM is unsaturated, pore fluids are oligotrophic, and microbial activity is limited under ambient conditions. Microbial activity in the near field during the postclosure period, when elevated temperatures prevail as a result of localized heating by the waste, will be even further inhibited by the drying of the tuff. Even if the tuff completely saturates as the repository cools, microbial activity will be limited because of the lack of nutrients. Thus, changes in porosity and permeability that could affect seepage, flow, and the repository's performance, because of the growth of microbes and the production of exopolymeric material as the near field evolves, are unimportant and need not be considered.

The potential importance of changes of pore-water and gas chemistry to repository performance is that mineral precipitation and dissolution is controlled by the composition of fluids. Calcite precipitation and dissolution are directly controlled by the partial pressure of CO_2 in equilibrium with pore fluids in the UZ. Volatilization of CO_2 as water evaporates is expected to increase gas phase CO_2 concentration to many times that of the ambient conditions (Lichtner, 1997). This increase has been observed in the drift-scale test at YM (unpublished results of Lawrence Berkeley National and Lawrence Livermore National Laboratories). Ambient gas chemistry appears controlled by near surface microbial processes (Thorstenson, et al., 1998). The CO_2 concentration in the gas phase as the near-field environment evolves will be controlled primarily by THC processes as a result of the fast kinetics of these processes and the oligotrophic nature of the tuffs at YM.

Based on the groundwater studies, organic C is expected to be limiting for microbial growth and activity. Nevertheless; it needs to be recognized that unknown, but limited, quantities of xenobiotic C will be introduced into the emplacement drifts (Haldeman, et al., 1996; Horn and Meike, 1995) during the preclosure operation of the repository. These xenobiotic compounds will include diesel fuel, lubricating oil, and other organic compounds associated with the operation of machinery (Haldeman, et al., 1996; Hardin and Chestnut, 1997). Current site characterization operations within the ESF (Wilder, 1996) and the Enhanced Characterization of the Repository Block Cross Drift include a spill program (CRWMS M&O, 1998a,b) that requires spill minimization and cleanup activities for spillage of organic fluids. While there is a tremendous taxonomic diversity of bacteria capable of using petroleum products as a C source, the limited quantity of water in the drifts (due to ventilation during the preclosure and radioactive decay heating in the postclosure) and the limited quantities of organic C added to the drifts should limit the potential importance of microbial activity to repository performance.

Additional insights on the potential importance of microbial processes in the near field can be derived from experiments designed to study the gross effects of microbial activity on repository geochemistry, radionuclide sorption, and integrity of repository and host rock materials (West, et al., 1998). Fermentation cells were loaded with carbon steel coupons, ion-exchange resins embedded in cement paste, cement-pumice composite blocks, and marl. The cells were then filled with fluids likely encountered in a potential Swiss repository and inoculated with a diverse mixture of microbes. The presence of microbes in these experiments did not appear to influence the overall geochemistry in any of the experiments, which was dominated by cement dissolution (West, et al., 1998). Geochemical modeling of the experiments could reproduce many of the observed features without explicitly invoking microbial activity, while discrepancies between the experiments and models were mostly explained by data or model limitations (West, et al., 1998).

Thus, changes in pore-water and gas chemistry because microbial activity that could affect seepage, flow, and the repository's performance, will be insignificant relative to chemical changes expected as a result of THC processes and interaction of engineered materials with the surrounding tuff. Therefore, the effects of microbial processes on seepage and flow need not be considered in a PA. Should the design of the repository change to one in which large quantities of organic carbon would be left in the emplacement drifts, then the potential for microbial activity that could affect seepage and flow would need to be reevaluated.

5.4.1 Subissue 1: Effects of Coupled Thermal-Hydrologic-Chemical Processes on Drift Seepage and Flow in the Unsaturated Zone

In the YMRP, the DOE approach to assess the effects of coupled THC processes on seepage and flow must meet the following model abstraction acceptance criteria for each relevant ISI: (i) integration; (ii) data and model justification; (iii) data uncertainty and verification; (iv) model uncertainty; and (v) model support. Quality assurance is handled in a separate section of the YMRP.

Three model abstraction ISIs are influenced by the ENFE within the scope of this flow subissue. The ISIs are (i) Spatial and Temporal Distribution of Flow, (ii) Quantity and Chemistry of Water Contacting Waste Packages and Waste Forms, and (iii) Flow Paths in the Unsaturated Zone (U.S. Nuclear Regulatory Commission, 2000a). The NRC TSPA Code uses these three abstractions (U.S. Nuclear Regulatory Commission, 2000a,b). The features and processes listed previously need to be considered in the evaluation of each abstraction. As part of this evaluation, the staff will use the acceptance criteria and review methods in the YMRP (U.S. Nuclear Regulatory Commission, 2000a) to review the DOE PMRs and the supporting AMRs as they become available. This evaluation will also include a review of the relevant FEPs included/excluded from the DOE TSPA.

The review will focus on a subset of the AMRs and PMRs that reflects the importance of the abstractions to the DOE safety case and relevance to ENFE Subissue 1. The following AMRs are a subset of those identified in the DOE AMRs/PMRs schedule as relevant to the ENFE subissue on seepage and flow: PMR on UZ Flow and Transport, U0075–AMR on Seepage Model for PA; N0120–AMR on Drift Scale Coupled Processes; U0120–AMR on Drift Seepage Including Coupled Processes; U0105–AMR on Mountain Scale Coupled Processes, and; N0080–FEPs for the Near-Field Environment.

Of the relevant AMRs and PMRs, only U0075 (CRWMS M&O, 2000b) and PMR-UZ (CRWMS M&O, 2000c), are available for review as of this writing. In the following sections, the resolution status is based on these two documents and the LADS report (CRWMS M&O, 1999a), the TSPA-SR Methods and Assumptions Report (CRWMS M&O, 1999b), and the Revision 3 of the Repository Safety Strategy (CRWMS M&O, 2000a). It is important to note that the TSPA-SR Methods and Assumption Report does not contain details on how the different modeling approaches will be implemented. The resolution status of this subissue will be further updated as more AMRs and PMRs become available for review.

To facilitate the discussion of the resolution status with respect to the effects of coupled THC processes on flow and transport, the acceptance criteria for the three relevant ISIs are listed in the following subsection. A summary of the DOE models, abstractions, and analyses relevant to seepage and UZ flow are presented in Section 5.4.1.2, and staff analyses of the DOE models, abstractions, and analyses are presented in Section 5.4.1.3.

5.4.1.1 Acceptance Criteria

The DOE approach to abstract coupled THC effects on seepage and flow in a TSPA for the proposed repository at YM will be acceptable provided that each of the acceptance criteria as described in the YMRP, Revision 0 (U.S. Nuclear Regulatory Commission, 2000a) are met for the ISIs on spatial and temporal distribution of flux, quantity and chemistry of water contacting WPs and waste forms, and flow paths in the UZ. These acceptance criteria pertain to (i) integration, (ii) data and model justification, (iii) data uncertainty and verification, (iv) model uncertainty, and (v) model verification. A description of these acceptance criteria, taken from the pertinent sections of the YMRP, are given in this section.

Criterion 1: Integration

ISI—Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms:

> Important design features, physical phenomena and couplings, and consistent and appropriate assumptions have been identified and described sufficiently for incorporation in to the abstraction of the quantity and chemistry of water contacting WPs and WFs in the PA and other related abstractions in the TSPA, and the technical bases are provided. The features, phenomena and couplings, and assumptions used to abstract the quantity and chemistry of water contacting WPs and WFs have been provided. The TSPA abstraction is consistent with the identification and description of those aspects of the quantity and chemistry of water contacting WPs and WFs that are important to waste isolation. The TSPA abstraction is also consistent with the technical bases for these descriptions of barriers important to waste isolation.

ISI—Spatial and Temporal Distribution of Flow:

> Important design features, site-specific physical phenomena and couplings, and consistent and appropriate assumptions have been incorporated into the spatial and temporal distribution of flow abstraction in the PA and the technical bases are provided. The TSPA abstraction in the DOE LA identifies and describes aspects of spatial and temporal distribution of flow that are important to waste isolation and includes the technical bases for these descriptions.

ISI—Flow Paths in the Unsaturated Zone:

> Important design features, physical phenomena and couplings, consistent and appropriate assumptions have been incorporated into the abstraction of flow paths in the UZ and other abstractions in the TSPA and the technical bases are provided. The TSPA abstraction in the DOE license application (LA) identifies and describes aspects of flow paths in the UZ that are important to waste isolation and includes the technical bases for these descriptions.

Criterion 2: Data and Model Justification

ISI—Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms:

> Sufficient data on design features (including drip shield, backfill, WPs, cladding, other EB components, and thermal loading), geology, hydrology, geochemistry, and geomechanics of the UZ and drift environment (e.g., field, laboratory, and natural analog

data) are available to adequately define relevant parameters and conceptual models necessary for developing the abstraction of the quantity and chemistry of water contacting WPs and WFs in the TSPA. The data are also sufficient to assess the degree to which FEPs related to the quantity and chemistry of water contacting WPs and WFs and which affect compliance with post-closure performance objectives have been characterized and to determine whether the technical bases provided for inclusion or exclusion of these FEPs are adequate. Where adequate data do not exist, other information sources such as expert elicitation have been appropriately incorporated into the abstraction process.

ISI—Spatial and Temporal Distribution of Flow:

Sufficient data (field, laboratory, and/or natural analog data) that are consistent with site characteristics are available to adequately define relevant parameters and conceptual models necessary for developing the spatial and temporal distribution of flow abstraction used in TSPA. The data are also sufficient to assess the degree to which FEPs related to the spatial and temporal distribution of flow and which affect compliance with 10 CFR 63.113(b) have been characterized and to determine whether the technical bases provided for inclusion or exclusion of these FEPs are adequate.

ISI—Flow Paths in the Unsaturated Zone:

Sufficient data (field, laboratory, and/or natural analog data) are available to define relevant parameters and conceptual models necessary for developing the TSPA abstraction of flow paths in the UZ, including the distribution of mass flux between fractures and matrix. The data are also sufficient to assess whether FEPs related to flow paths in the UZ that affect compliance with10 CFR 63.113(b) have been adequately characterized, and whether the technical bases provided for inclusion or exclusion of these FEPs are adequate.

Criterion 3: Data Uncertainty and Verification

ISI—Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms:

Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the TSPA abstraction of quantity and chemistry of water contacting WPs and WFs, such as the pH, chloride concentration, and amount of water flowing in and out of the breached WP, are consistent with site characterization data, design data, laboratory experiments, field measurements, and natural analog data, are technically defensible, and reasonably account for uncertainties and variabilities. The technical bases for the parameter values used in the TSPA abstraction are provided.

ISI—Spatial and Temporal Distribution of Flow:

Determine that parameter values, assumed ranges, probability distributions, and/or bounding assumptions used in the spatial and temporal distribution of flow abstraction are consistent with site characterization data, are technically defensible, and reasonably account for uncertainties and variabilities. The technical bases for the parameter values used in the PA have been provided.

ISI—Flow Paths in the Unsaturated Zone:

Parameter values, assumed ranges, probability distributions, and/or bounding assumptions used in the abstraction of flow paths in the UZ, including the distribution of mass flux between fractures and matrix, are technically defensible and reasonably account for uncertainties and variabilities. The technical basis for the parameter values used in the PA is provided.

Criterion 4: Model Uncertainty

ISI—Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms:

Alternative modeling approaches consistent with available data (e.g., design features, field, laboratory, and natural analog) and current scientific understanding are investigated and results and limitations are appropriately factored into the abstraction of quantity and chemistry of water contacting WPs and WFs. DOE has provided sufficient evidence that ACMs of FPs have been considered, that the models are consistent with available data and current scientific understanding, and that the effect of these ACMs on TSPA has been evaluated.

ISI—Spatial and Temporal Distribution of Flow:

Alternative modeling approaches consistent with available data and current scientific understanding are investigated and results and limitations are appropriately factored into the spatial and temporal distribution of flow abstraction. DOE has provided sufficient evidence that ACMs of FEPs have been considered, that the models are consistent with available data (e.g., field, laboratory, and natural analog) and current scientific understanding, and that the effect of these ACMs on TSPA has been evaluated.

ISI—Flow Paths in the Unsaturated Zone:

Alternative modeling approaches, consistent with available data and current scientific understanding, are investigated and results and limitations appropriately factored into the abstraction of flow paths in the UZ, including the distribution of mass flux between matrix and fractures. DOE has provided sufficient evidence that ACMs of FPs have been considered, that the models are consistent with available data (e.g., field, laboratory, and natural analog) and current scientific understanding, and that the effect of these ACMs on TSPA has been evaluated.

Criterion 5: Model Verification

ISI—Quantity and Chemistry of Water Contacting the Waste Packages and Waste Forms:

Output from the TSPA abstraction of quantity and chemistry of water contacting WPs and WFs is justified through comparison with output from detailed process-level models and/or empirical observations (e.g., laboratory testing, field measurements, natural analogs).

ISI—Spatial and Temporal Distribution of Flow:

Output from the TSPA abstraction of the spatial and temporal distribution of flow is verified through comparison with output from detailed process-models and/or empirical observations (laboratory and field testings or natural analogs, or both).

ISI—Flow Paths in the Unsaturated Zone:

TSPA code output of the distribution of flow paths in the UZ, including the mass flux between matrix and fracture abstraction, is verified through comparison with detailed process models and/or empirical observations (e.g., laboratory testing, field measurements, and natural analogs).

5.4.1.2 Description of the U.S. Department of Energy Models, Abstractions, and Analyses

According the Repository Safety Strategy, "principal factors" are central to determining and demonstrating long-term safety of the repository system, and will be the focus of postclosure safety considerations for the SR and LA decisionmaking. Three of the principal factors that were identified by the DOE for the enhanced repository system are potentially affected directly by THC-induced changes to flow properties: (i) limited seepage of water into the emplacement drifts, (ii) retardation of radionuclide migration in the UZ, and (iii) dilution of radionuclide concentrations during migration. The TSPA-SR Methods and Assumptions Report (CRWMS M&O, 1999b) outlines how these factors will be addressed by abstractions and process-level models in the TSPA-SR and LA to provide the technical basis for the postclosure safety case.

A major assumption embedded in the TSPA-VA was that coupled THC effects were of a transient nature and would not result in long-term changes to rock flow properties. DOE has taken significant steps to develop technical support for this assumption for the reports supporting the LA and the TSPA-SR. In particular, abstractions and process-level models are being refined to take into account the potential effects of the new repository design and to improve THC models. THC effects on flow are treated in a series of sensitivity analyses. The results of these sensitivity analyses will be used to update hydrological properties in abstractions of relevant processes, where appropriate.

The following subsections provide additional information on DOE treatment of individual physical processes that form components of the DOE "principal factors" and are also potentially affected by THC induced-changes to flow properties. This summary is organized around the three ISIs affected by ENFE Subissue 1 and is based on the Repository Safety Strategy, the SR Methods and Assumptions Document, and the Unsaturated Zone Flow and Transport PMR. Supporting AMRs are not available for review at this writing. The focus is on those concerns relevant to the ENFE Subissue 1; additional information about these UZ flow concerns is provided in the USFIC IRSR.

5.4.1.2.1 Spatial and Temporal Distribution of Flow

This model abstraction ISI is concerned with the spatial and temporal distribution of percolation flux reaching the repository horizon, which is potentially altered by persistent THC-induced changes to rock properties. This model abstraction ISI overlaps with the ISI on Quantity and Chemistry of Water Contacting the Waste Package on the topic of seepage into the drift. Drift seepage is considered in the following section. The discussion here focuses on THC effects on UZ flow above the emplacement drifts, which sets the boundary conditions for the drift seepage. Detailed discussions of the various processes comprising this ISI can be found in the IRSR for the USFIC KTI.

The approach in the TSPA-SR for flow in the UZ is similar to that used in the TSPA-VA. That is, a calibrated three-dimensional (3D) mountain-scale flow model was developed, based on the dual-permeability formulation for fracture/matrix flow with the active-fracture model, to describe the reduced coupling between fractures and matrix expected under unsaturated conditions.

Hydrological properties used in the model were obtained by inverse modeling to match measured liquid saturations and other hydrological variables. These data were obtained in the ambient system, which has not been altered by repository-induced THC effects. THC effects on flow above the repository were not considered in the UZ flow model; instead, THC models were used in sensitivity studies to demonstrate that bulk changes in hydrological properties are minor for the ranges of thermal loadings used in the EDA-II design.

The supporting THC simulations (CRWMS M&O, 2000c) used the active-fracture dual-continuum formulation for two-phase, nonisothermal flow and chemical transport. The domain of the two-dimensional model extended vertically from the surface to the Calico Hills unit. Horizontally, the model domain spanned one-half of the drift spacing. An unstructured grid with refinements around the drift was used. Equations describing heat, liquid and gas flow, chemical transport, chemical reactions, and porosity and permeability changes were solved sequentially using TOUGHREACT V2.2. Two chemical systems were considered, one with a simplified representation of the mineralogy (silica phases, gypsum, and calcite) and a second with a large number of minerals including those representative of the likely secondary phases formed from thermal alterations of zeolitic units. Geochemical data on mineral abundances and compositions, reaction rates, and water compositions were taken from various sources.

Results of both models show precipitation of calcite in the fracture system in an extended area because of the increase in temperature and the retrograde solubility of calcite. Silica redistribution was confined to regions of limited spatial extent, mostly associated with the position of the boiling front. In all cases, the change in porosity caused by these processes was small compared with the initial porosity. Resulting changes in hydrological properties are expected to be negligible. These results are in stark contrast to modeling results performed in support of the TSPA-VA, which showed the formation of a robust mineralized cap with reduced permeability above the repository. The reduced THC alteration associated with the EDA-II design is a consequence of the increased drift spacing and lower overall heat loading.

The PMR-UZ also contains a discussion on the possibility of matrix sealing by precipitation of silica in a highly localized zone at the fracture-matrix interface. It is argued that the potential for this probably to occur is small because the kinetic rates for silica dissolution and the silica concentration in the fractures are small. No values are provided for any of these parameters. Theoretical studies by Lichtner, Keating, and Carey (1999) clearly show that the effect is possible and may proceed rapidly relative to the duration of the thermal pulse with some combinations of these parameters. It was also argued that there is little hydrological potential for flow from fractures to matrix, a statement that clearly neglects the strong imbibition from fractures to matrix that exists with some saturation conditions.

The potential for thermal alteration of volcanic glasses in the Paintbrush Tuff unit was also addressed in sensitivity studies. The flow fields developed for the TSPA-SR do not allow for possible mineralogical phase changes from volcanic glasses to zeolites and clays. Instead, mountain-scale TH models were used to calculate temperatures in this unit. The temperatures within the Paintbrush Tuff were calculated to be in the range of 40–45 °C with ventilation. Without ventilation, the base of the Paintbrush Tuff reached temperatures of 70–75 °C; in areas of low infiltration, the temperatures at the base of the Paintbrush Tuff reached boiling conditions. The PMR provides no technical basis for ignoring possible alterations of glasses at these elevated temperatures.

5.4.1.2.2 Quantity and Chemistry of Water Contacting Waste Packages

Drift seepage is an important control on the amount of water contacting the WP and is potentially altered by THC effects. The approach proposed for drift seepage in the TSPA-SR is similar to that used in the TSPA-VA. Probability distributions are defined for the fraction of WPs wetted by seepage and for the flow rate in the seeps. These distributions are based on detailed modeling of capillary diversion around the emplacement drifts, as described in U0075–AMR on Drift Seepage Model for PA.

The drift seepage models used Richard's equation to describe unsaturated flow around the emplacement drifts. The fracture system was treated as an equivalent continuum; flow in the matrix was neglected. The fracture permeability, which is expected to exhibit a high degree of spatial variability, was treated as a random space function. A small number (3–5) of realizations was created for this random permeability field using standard geostatistical techniques. Each realization was then used in the solution of Richard's equation to determine a seepage fraction and seep rate. The average permeability for the fracture system was based on air-permeability measurements, representative of ambient conditions (i.e., unaltered by coupled THC processes). This average fracture permeability was varied for a range of three orders of magnitude to assess sensitivities to this uncertain parameter. The van Genuchten parameter $1/\alpha$, which quantifies the strength of moisture retention in the unsaturated fracture system, was treated as spatially constant except for a small number of sensitivity runs, where it was considered related deterministically to the spatially variable fracture permeability. The value of

$1/\alpha$ was varied 30–1000 Pa, which spans the range observed in the ambient system. Other relevant parameters also were considered in the sensitivity studies, including the spatial correlation range, and the variance in ln k_f, where k_f is the fracture permeability. The simulations show that drift seepage decreases with increasing fracture permeability and increasing $1/\alpha$. Weaker sensitivity was noted to the variance in ln k_f and to the spatial correlation range. In general, drift seepage increases with increasing correlation range and increasing ln k_f variance.

The potential effects of THC alteration of fracture properties on drift seepage are ignored in the abstractions for the TSPA-SR. This neglect is based on fully coupled THC simulations, which show negligible alteration of the fracture and matrix porosities. These simulations are described in the previous section. The reduced degree of mineral precipitation and dissolution associated with the EDA-II design is a consequence of the reduced thermal loading.

The Repository Safety Strategy also outlines an alternative approach to drift seepage being considered by DOE. This new approach is based on the concept of a seepage threshold—a value of percolation flux below which seepage does not occur. The approach outlined in the Repository Safety Strategy involves determining the seepage threshold from *in situ* measurements. The empirically determined threshold would then be used in PA calculations; that is, drift seepage would not be considered in subareas of the repository where the percolation flux is below the threshold. In practice, this means that seepage will be allowed only in regions of extreme flow. At this writing, few details are available on the seepage threshold approach. In particular, it is unclear how the DOE plans to justify the neglect of persistent THC-induced changes in rock properties in this approach.

5.4.1.2.3 Flow Paths in the Unsaturated Zone

The approach prepared for TSPA-SR for flow in the UZ is similar to that used in the TSPA-VA. That is, flow fields obtained by 3D mountain-scale flow models for discrete cases are used as input into transport models without further abstraction. The flow model is based on the dual-permeability formulation for fracture/matrix flow with the active-fracture model to describe the reduced coupling between fractures and matrix expected under unsaturated conditions. Partitioning between the matrix and fracture system is important because flow through the fractures is rapid compared to flow through the matrix and because sorption on minerals is expected to retard radionuclide movement in the matrix but not in the fractures. Hydrological properties used in the model are to be obtained by inverse modeling to match observed data in the ambient (unaltered by THC effects) system. The flow model/abstraction was not modified to consider mineral precipitation or dissolution near the repository drifts. Instead, fully coupled THC simulations were used to show that the resulting porosity changes are negligible. These simulations are described in Section 5.4.1.2.1.

Radionuclide travel time to the water table is strongly controlled by the Calico Hills nonwelded unit. Significant lateral diversion may occur in and above this unit, as indicated by observed regions of perched water. Pathways through the Calico Hills nonwelded unit are controlled by the highly heterogeneous fracture and matrix permeabilities in this unit and by discrete features such as faults. The Calico Hills unit is susceptible to hydrothermal alteration. In particular, the remaining volcanic glass in this unit may be altered to lower permeability zeolites, with important potential consequences for groundwater travel time. This potential alteration was not included in the flow model and abstraction. Expected temperatures at the top of the Calico Hills units were calculated using dual-permeability hydrothermal models to reach a maximum of 70–75 °C during the period of 2000–7000 yr after closure. A technical basis for neglected thermal alterations at these elevated temperatures was not provided in the Unsaturated Zone Flow and Transport PMR. The supporting AMRs are not available for review as of this writing.

5.4.1.3 Analysis of the U.S. Department of Energy Models, Abstractions, and Analyses

Most of the AMRs that provide the details on DOE models, abstractions, and analyses are not available as of this writing. The following sections focus on the abstraction architecture described in the Repository Safety Strategy, the TSPA-SR Methods and Assumptions Report (CRWMS M&O, 1999b), and the summary provided in the Unsaturated Zone Flow and Transport PMR. For this revision of the ENFE IRSR, staff analysis focused on the acceptance criterion on integration. Staff analysis using all five acceptance criteria will be completed as the DOE AMRs become available. An analysis of the FEPs relevant to Subissue 1 of the ENFE IRSR is presented in the first part of this section, followed by discussions specific to the three ISI model abstractions.

5.4.1.3.1 Features, Events, and Processes Screening

A formal screening process for FEPs was not developed for the TSPA-VA, and many important design features, physical phenomena, and couplings were not evaluated in a PA framework. The DOE since has developed a formal documentation of the FEPs identification and screening processes in preparation for the TSPA-SR. The DOE identification, screening, and documentation processes for FEPs are expected to consider known temporal and spatial variations in conditions affecting coupled THC effects on seepage and flow and to relay this information in a thorough and transparent manner if the FEPs can not be excluded from further consideration.

The contents of the DOE FEPs database (Swift, et al., 1999) have been screened to identify FEPs related to the ENFE subissue on seepage and flow (Pickett and Leslie, 1999; U.S. Nuclear Regulatory Commission, 2000b). The audit review of Pickett and Leslie (1999) indicated that 58 primary FEPs are relevant to ENFE Subissue 1. In further review of the FEPs database, staff identified one additional FEPs (2.2.08.03.00–Geochemical interactions in geosphere) relevant to the seepage and flow subissue. This additional review also removed five FEPs from the Pickett and Leslie (1999) list of FEPs relevant to the ENFE Subissue 1: 2.1.01.03.00 Heterogeneity of Waste Forms, 2.3.13.03.00 Effects of Repository Heat on Biosphere, 2.2.07.14.00 Density Effects on Groundwater Flow, and 2.2.10.08 Thermo-Chemical Alteration of the Saturated Zone.

Of the primary FEPs relevant to Subissue 1, 17 are excluded by the DOE screening process, and 2 have no determination listed. In the audit review of Pickett and Leslie (1999), it was determined that 15 of the excluded 17 FEPs have inadequate or missing screening arguments. Staff reviewed in more detail the other 2 excluded FEPs and agree with the DOE disposition of these, based on screening arguments presented in the FEPs database (Swift, et al., 1999). No further analysis of the relevance of these FEPs to the ENFE Subissue 1 is anticipated.

Table 5-1 lists primary FEPs relevant to ENFE Subissue 1 and indicates the corresponding ISI affected by each. This list includes FEPs to be included in the TSPA-SR and those excluded but determined to have inadequate screening arguments. In addition, Pickett and Leslie (1999) identified two FEPs relevant to ENFE Subissue 1 but not included in the FEPs database. Both of these FEPs are concerned with dehydration reactions. The first of these missing FEPs is dehydration of zeolites below the repository. Dehydration could result in large-scale volume changes thereby affecting porosity and, indirectly, flow paths. The second FEPs is concerned with direct alteration of flow because of water released from mineralogic dehydration reactions. Both of these FEPs potentially affect the model abstraction ISI on Flow Paths in the Unsaturated Zone. Technical bases should be provided for exclusion of these FEPs from consideration in the SR and LA.

5.4.1.3.2 Spatial and Temporal Distribution of Flow

Coupled THC processes that might affect the spatial and temporal distribution of flow above the emplacement drifts were omitted without technical justification in the TSPA-VA. The DOE has taken significant steps toward addressing these potential effects in the Unsaturated Zone Flow and Transport PMR. Staff agree that the general approach—to use sensitivity analyses to show that the hydrological parameters are not significantly affected by THC processes—is an appropriate one.

Coupled THC simulations undertaken to support the UZ flow and transport model show that maximum porosity change caused by mineral precipitation and dissolution is on the order of 1 percent of the initial porosity. Such a small change in porosity is expected to have negligible effects only on bulk hydrological properties. The model used in the analysis is near state-of-the-art and appropriate for the task of addressing bulk property modification. Data justification, data uncertainty, model uncertainty, and model verification were not reviewed because the supporting AMR is not available at this writing. If future reviews by the staff determine these acceptance criteria are also met, then DOE neglect of the effect of mineral precipitation and dissolution on bulk hydrological parameters used in determining the spatial and temporal distribution of flow would be acceptable.

Although the DOE THC model is appropriate for addressing the concern of bulk property modification caused by mineral precipitation and dissolution, it is not an appropriate model for addressing the formation of a highly localized low-permeability zone caused by mineral precipitation at the interface between fractures and matrix. Such sealing of the matrix might lead to significant hydrological changes by decoupling the matrix and fracture systems, even if the overall change in porosity is small. The DOE treatment of this effect in the PMR on Unsaturated Zone Flow and Transport is limited to a nonquantitative discussion and does not represent an adequate technical basis for omission in the TSPA. In particular, the DOE argument hinges on low kinetic rates for silica precipitation in the welded units and on a presumption of low silica concentrations in the fractures, yet no values for these parameters are provided. This approach does not meet the acceptance criteria on data justification and data uncertainty. Further, the

Table 5-1. U.S. Department of Energy features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to Subissue 1 of the Evolution of the Near-Field Environment Key Technical Issue (Pickett and Leslie, 1999). The X shows which U.S. Nuclear Regulatory Commission model abstraction integrated subissues are relevant to the FEPs.

Features, Events, and Processes Number	Features, Events, and Processes Name	Screening	Spatial and Temporal Distribution of Flux	Quantity and Chemistry of Water	Flow Paths in the Unsaturated Zone
1.1.02.00.00	Excavation/construction	Exclude	X	X	X
1.1.02.02.00	Effects of preclosure ventilation	??	X		X
1.1.03.01.00	Error in waste or backfill emplacement	Exclude		X	
1.1.07.00.00	Repository design	Include (exclude deviations from design)	X	X	X
1.1.08.00.00	Quality control	Include (exclude defects and deviations)	X	X	X
1.1.12.01.00	Accidents and unplanned events during operation	Exclude	X	X	X
1.1.13.00.00	Retrievability	Include	X	X	X
1.2.02.01.00	Fractures	Include (existing, reactivated), Exclude (new, SZ)	X	X	X
1.2.04.02.00	Igneous activity causes changes to rock properties	Include	X	X	X
1.2.06.00.00	Hydrothermal activity	Exclude	X	X	X
1.2.08.00.00	Diagenesis	Exclude	X		X
2.1.01.02.00	Codisposal/colocation of waste	Include	X	X	X

Table 5-1. U.S. Department of Energy features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to Subissue 1 of the Evolution of the Near-Field Environment Key Technical Issue (Pickett and Leslie, 1999). The X shows which U.S. Nuclear Regulatory Commission model abstraction integrated subissues are relevant to the FEPs. (cont'd)

Features, Events, and Processes Number	Features, Events, and Processes Name	Screening	Spatial and Temporal Distribution of Flux	Quantity and Chemistry of Water	Flow Paths in the Unsaturated Zone
2.1.02.08.00	Pyrophoricity	Exclude	X	X	X
2.1.04.01.00	Preferential pathways in the backfill	Include		X	
2.1.04.02.00	Physical and chemical properties of backfill	Include		X	
2.1.04.03.00	Erosion or dissolution of backfill	Exclude		X	X
2.1.04.05.00	Backfill evolution	Include		X	X
2.1.05.01.00	Seal physical properties	Include	X	X	
2.1.05.03.00	Seal degradation	Include		X	X
2.1.06.01.00	Degradation of cementitious materials in drift	Include		X	X
2.1.06.02.00	Effects of rock reinforcement materials	Include	X	X	X
2.1.06.03.00	Degradation of the liner	Include		X	X
2.1.06.04.00	Flow through the liner	Exclude		X	X
2.1.06.05.00	Degradation of invert and pedestal	Include			X
2.1.06.06.00	Effects and degradation of drip shield	unspecified			X
2.1.06.07.00	Effects at material interfaces	Include			X
2.1.08.01.00	Increased unsaturated water flux at the repository	Include		X	X
2.1.08.02.00	Enhanced influx (Philip's drip)	Include		X	X
2.1.08.04.00	Condensation forms on backs of drifts	Include		X	

Table 5-1. U.S. Department of Energy features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to Subissue 1 of the Evolution of the Near-Field Environment Key Technical Issue (Pickett and Leslie, 1999). The X shows which U.S. Nuclear Regulatory Commission model abstraction integrated subissues are relevant to the FEPs. (cont'd)

Features, Events, and Processes Number	Features, Events, and Processes Name	Screening	Spatial and Temporal Distribution of Flux	Quantity and Chemistry of Water	Flow Paths in the Unsaturated Zone
2.1.08.05.00	Flow through invert	Include			X
2.1.08.08.00	Induced hydrological changes in the waste and EBS	Include		X	X
2.1.08.11.00	Resaturation of repository	Include	X	X	X
2.1.09.12.00	Rind (altered zone) formation in waste, EBS, and adjacent rock	Include	X	X	X
2.1.11.02.00	Nonuniform heat distribution/edge effects in repository	Include	X	X	X
2.2.01.02.00	Thermal and other waste and EBS-related changes in the adjacent host rock	Include	X	X	X
2.2.01.03.00	Changes in fluid saturations in the EDZ	Include	X	X	X
2.2.03.02.00	Rock properties of host rock and other units	Include	X	X	X
2.2.07.05.00	Flow and transport in the UZ from episodic infiltration	Include	X	X	X
2.2.07.06.00	Episodic/pulse release from repository	?	X	X	X
2.2.07.07.00	Perched water develops	Exclude	X		X
2.2.07.10.00	Condensation zone forms around drifts	Include	X	X	
2.2.07.11.00	Return flow from condensation cap/resaturation of dryout zone	Include	X	X	
2.2.07.15.06	Convection (water transport)	Exclude		X	X

Table 5-1. U.S. Department of Energy features, events, and processes (FEPs) database (Revision 00b) (U.S. Department of Energy, 1999) entries relevant to Subissue 1 of the Evolution of the Near-Field Environment Key Technical Issue (Pickett and Leslie, 1999). The X shows which U.S. Nuclear Regulatory Commission model abstraction integrated subissues are relevant to the FEPs. (cont'd)

Features, Events, and Processes Number	Features, Events, and Processes Name	Screening	Spatial and Temporal Distribution of Flux	Quantity and Chemistry of Water	Flow Paths in the Unsaturated Zone
2.2.07.15.07	Dispersion (water transport)	Include		X	X
2.2.08.01.00	Groundwater chemistry/composition in UZ and SZ	Include	X	X	X
2.2.10.01.00	Repository-induced thermal effects in geosphere	Include	X	X	X
2.2.10.06.00	Thermo-chemical alteration (solubility, speciation, phase changes, precipitation/dissolution)	Include	X	X	X
2.2.10.07.00	Thermo-chemical alteration of the Calico Hills unit	Include			X
2.2.10.09.00	Thermo-chemical alteration of the Topopah Spring basal vitrophyre	Include			X
2.2.10.10.00	Two-phase buoyant flow/heat pipes	Include	X		X
2.2.10.11.00	Natural airflow in UZ	Include	X	X	X
2.2.10.12.00	Geosphere dryout due to waste heat	Include	X		X
2.2.11.01.05	Gas generation and gas sources, far-field	Exclude	X		X
2.2.11.02.00	Gas pressure effects	Exclude	X		X
3.1.01.01.00	Radioactive decay and ingrowth	Include	X	X	X

SZ = saturated zone EBS = engineered barrier system
UZ = unsaturated zone EDZ = excavation disturbed zone

PMR-UZ also argues there is little hydrological potential for flow from fractures to matrix under unsaturated conditions, an argument clearly incorrect given the strong imbibition from fractures to matrix that can exist under some saturation conditions. If this process is neglected in the TSPA-SR, DOE should either show that the effect is unimportant for performance or provide a sound technical basis for neglecting the effect using data appropriate for the expected conditions.

The DOE TH calculations show that the base of the Paintbrush Tuff may approach boiling conditions in situations of low infiltration. The Paintbrush Tuff is susceptible to thermal alteration and also plays a potentially important role in the hydrology system by dampening large infiltration events. No technical bases were provided for neglecting the potential alterations to the Paintbrush Tuff. To meet Criterion 1 on Integration, DOE should provide the technical bases for neglect of thermal alteration of the Paintbrush Tuff, demonstrate that the alteration is unimportant to performance, or incorporate the effect of the alterations into future abstractions of spatial and temporal distribution of flow.

5.4.1.3.3 Quantity and Chemistry of Water Contacting Waste Packages

Coupled THC processes have the potential for producing significant persistent changes to the rock flow properties in the immediate vicinity of the host rock during the 10,000 yr compliance period, thereby affecting seepage into the drifts. Coupled THC processes that might affect seepage were not considered explicitly in the TSPA-VA (U.S. Department of Energy, 1998b). The approach for the SR is to use auxiliary analyses to demonstrate that THC effects will not alter hydrological properties beyond the range used in the PA abstractions. In broad terms, staff agree this is an appropriate plan for addressing the subissue.

Coupled THC simulations undertaken to support the drift seepage model show that THC-induced changes in bulk porosity are small. Within a continuum-level framework, the resulting changes in permeability and moisture retention properties would also be small. Data justification, data uncertainty, model uncertainty, and model verification were not reviewed because the supporting AMR is not available at this writing. If future review by the staff determines these acceptance criteria are also met, then DOE neglect of bulk hydrological property changes because of mineral precipitation and dissolution would be acceptable. It is acceptable also to neglect the formation of a localized low-permeability layer at the fracture-matrix interface, provided DOE continues to base the seepage abstraction on a single-continuum (fracture only) model for seepage. If, however, future DOE approaches to drift seepage take credit for the beneficial effects of the matrix, then the topic of matrix sealing should be addressed more carefully, as discussed in the previous section. For example, if an empirically determined drift-seepage threshold, which implicitly takes credit for matrix effects in controlling drift seepage, is used in the TSPA-SR, then the topic of matrix sealing needs to be revisited.

In the DOE abstraction of seepage into drifts, the seepage flow rate was increased by a factor of 1.5, in part to account for increased seepage along rock bolts. Increased seepage along rock bolts might occur, for example, because of localized chemical interaction between the cementitious grout and the surrounding tuff rock. DOE should provide a justification why this factor of 1.5 is conservative.

5.4.1.3.4 Flow Paths in the Unsaturated Zone

Coupled THC processes that might affect flow below the repository were not considered explicitly in the TSPA-VA (U.S. Department of Energy, 1998). The approach for the SR is to use auxiliary analyses to demonstrate that THC effects will not alter hydrological properties beyond the range used in the PA abstractions. This approach represents a significant step forward compared with the VA, and staff agree this is an appropriate approach to the subissue.

DOE coupled THC modeling shows significant changes in bulk hydrological parameters below the drift are unlikely. Data justification, data uncertainty, model uncertainty, and model verification were not reviewed because the supporting AMR is not available at this writing. If future reviews by the staff determines these acceptance criteria are also met, then the DOE neglect of bulk hydrological property changes caused by silica redistribution below the repository would be acceptable.

The DOE evaluation of the possibility for THC-induced matrix sealing does not meet the acceptance criteria for this ISI for the reasons described in Section 5.4.1.3.2. Formation of such a mineralized boundary layer has the potential to isolate fractures from the matrix, thereby forcing the majority of flow into the fractures. DOE should evaluate the potential for matrix sealing to affect repository performance. The clearest path to resolution on this concern may be simply to ignore matrix flow for a limited region below the drifts as a conservative bounding approximation. If the effect is neglected in the TSPA-SR, then a more quantitative supporting argument, based on data relevant to the expected repository conditions, should be put forward.

The Unsaturated Zone Flow and Transport PMR contains no discussion of the potential effects of cementitious material on the flow paths below the repository. Staff agree that the potential for hydrological changes resulting from chemical interactions between tuff rock and cementitious material is reduced greatly because of the limited use of cementitious materials in the EDA-II design. There is still a large amount of concrete proposed for the ventilation tunnels and shafts. Much of this concrete will experience elevated temperatures for long periods, with significant potential for chemical interaction with the adjacent tuff rock. An evaluation of the potential for cementitious materials to alter repository performance by altering hydrological properties below the repository is required before the ENFE Subissue 1 can be resolved. DOE indicates (Brocoum, 2000) this FEPs will be considered in the SR. Staff will review this effort when it becomes available.

The DOE dismisses the possibility for further hydrothermal alteration of the Calico Hills nonwelded unit by calculating temperatures there and arguing that these are below the critical temperature needed for significant alteration. No supporting data for the reaction rates at the calculated temperatures are provided or cited. Staff will review the supporting AMRs when they become available to determine if the necessary supporting data are provided.

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