Shale Disposal of U.S. High-Level Radioactive Waste

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Abstract

This report evaluates the feasibility of high-level radioactive waste disposal in shale within the United States. The U.S. has many possible clay/shale/argillite basins with positive attributes for permanent disposal. Similar geologic formations have been extensively studied by international programs with largely positive results, over significant ranges of the most important material characteristics including permeability, rheology, and sorptive potential. This report is enabled by the advanced work of the international community to establish functional and operational requirements for disposal of a range of waste forms in shale media. We develop scoping performance analyses, based on the applicable features, events, and processes identified by international investigators, to support a generic conclusion regarding post-closure safety. Requisite assumptions for these analyses include waste characteristics, disposal concepts, and important properties of the geologic formation. We then apply lessons learned from Sandia experience on the Waste Isolation Pilot Project and the Yucca Mountain Project to develop a disposal strategy should a shale repository be considered as an alternative disposal pathway in the U.S.

Disposal of high-level radioactive waste in suitable shale formations is attractive because the material is essentially impermeable and self-sealing, conditions are chemically reducing, and sorption tends to prevent radionuclide transport. Vertically and laterally extensive shale and clay formations exist in multiple locations in the contiguous 48 states. Thermal-hydrologic-mechanical calculations indicate that temperatures near emplaced waste packages can be maintained below boiling and will decay to within a few degrees of the ambient temperature within a few decades (or longer depending on the waste form). Construction effects, ventilation,

and the thermal pulse will lead to clay dehydration and deformation, confined to an excavation disturbed zone within a few meters of the repository, that can be reasonably characterized. Within a few centuries after waste emplacement, overburden pressures will seal fractures, resaturate the dehydrated zones, and provide a repository setting that strongly limits radionuclide movement to diffusive transport. Coupled hydrogeochemical transport calculations indicate maximum extents of radionuclide transport on the order of tens to hundreds of meters, or less, in a million years. Under the conditions modeled, a shale repository could achieve total containment, with no releases to the environment in undisturbed scenarios. The performance analyses described here are based on the assumption that long-term standards for disposal in clay/shale would be identical in the key aspects, to those prescribed for existing repository programs such as Yucca Mountain.

This generic repository evaluation for shale is the first developed in the United States. Previous repository considerations have emphasized salt formations and volcanic rock formations. Much of the experience gained from U.S. repository development, such as seal system design, coupled process simulation, and application of performance assessment methodology, is applied here to scoping analyses for a shale repository. A contemporary understanding of clay mineralogy and attendant chemical environments has allowed identification of the appropriate features, events, and processes to be incorporated into the analysis. Advanced multi-physics modeling provides key support for understanding the effects from coupled processes. The results of the assessment show that shale formations provide a technically advanced, scientifically sound disposal option for the U.S.

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Acronyms

AL ANDRA AR ASC AZ	Alabama Agence Nationale pour la Gestion Des Déchets Radioactifs (The French National Radioactive Waste Management Agency) Arkansas Advanced Simulation and Computing Arizona
BDCF	Biosphere dose conversion factor
BWR	Boiling water reactor
CO	Colorado
CSNF	Commercial spent nuclear fuel
DOE	U.S. Department of Energy
DSNF	DOE-owned defense spent nuclear fuel
EBS	Engineered barrier system
EDZ	Excavation damage zone
EIS	Environmental impact statement
ELWS	Estimated limiting waste stream
EPA	U.S. Environmental Protection Agency
FEPs	Features, events, and processes
FL	Florida
HADES HLW HLWG	High Activity Disposal Experimental Site (Underground laboratory in the Boom clay near Mol, Belgium) High-level waste High-level waste glass
IA	Iowa
IAEA	International Atomic Energy Agency
ICRP	International Commission on Radiation Protection
ID	Idaho
IL	Illinois
IRG	Interagency Review Group
KS	Kansas
LA	Louisiana
LaBS	Lanthanum borosilicate glass waste form
LPG	Liquified petroleum gas

Acronyms (Continued)

MI	Michigan
MOX	Mixed oxide (fuel)
MS	Mississippi
MT	Montana
MTHM	Metric tons of heavy metal
NAGRA	Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle (The Swiss National Cooperative for the Disposal of Radioactive Waste)
NC	North Carolina
ND	North Dakota
NEPA	National Environmental Policy Act (1970)
NM	New Mexico
NRC	U.S. Nuclear Regulatory Commission
NTS	Nevada Test Site
NWPA	Nuclear Waste Policy Act (1984, 1987)
NV	Nevada
NY	New York
ОН	Ohio
OK	Oklahoma
ONDRAF/	Oktanonia
NIRAS	l'Organisme national des déchets radioactifs et des matières fissiles enrichies
MIKAS	(Agency for Radioactive Waste and Enriched Fissile Materials, Belgium)
OR	Oregon
ORNL	Oak Ridge National Laboratory
D۸	Derformen en esseenment
PA	Performance assessment
PWR	Pressurized water reactor
R&D RMEI	Research and development Reasonably maximally exposed individual
	reasonably maximum exposed marriadur
SNF	Spent nuclear fuel
THC THMC TRU TX	Thermal-hydrologic -chemical Thermal-hydrologic-mechanical-chemical Transuranic (waste) Texas
UT UNF UOX URL	Utah Used nuclear fuel Uranium oxide (fuel) Underground research laboratory

Acronyms (Continued)

WAWashingtonWIPPWaste Isolation Pilot PlantWYWyomingYMPYucca Mountain Project

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1. INTRODUCTION

This report analyzes the technical features and safety performance of a repository for high-level radioactive waste (HLW, here used to include used nuclear fuel – UNF) in suitable clay or shale formations, in the United States. Because U.S. efforts have focused on the volcanic tuff site at Yucca Mountain, radioactive waste disposal in U.S. shale formations has not been considered for many years. However, advances in multi-physics computational modeling and research into clay mineralogy continue to improve the scientific basis for assessing nuclear waste repository performance in such formations. Importantly, several countries have actively studied nuclear waste disposal in clay/shale/argillite media for decades. The analysis reported here, although generic, draws heavily on extensive information from international repository programs that have continued to advance repository concepts in clay/shale.

Various references to lithology, or types of geologic formations, are used in this report. Potentially suitable mudstone, clay, shale, and argillite formations share many characteristics favorable to repository development and waste isolation. The lithologies represented by the several international sites cover a range of classifications, encompassing a broad range of material properties. For this report we refer to clay/shale media, intending to represent the full range of potentially suitable formations.

The primary countries considering clay/shale media for disposal of HLW are Belgium (plastic clay), France (argillite), and Switzerland (claystone). The geologic settings have been found sufficiently suitable that these repository programs have matured to include production of results from *in situ* tests performed in underground research laboratories, with corresponding refinement of repository design concepts, and medium-specific performance analyses. For this generic evaluation, design and operational concepts from these international programs are used as the design basis. This use of existing work permits a credible analysis that applies to the many clay/shale formations in the U.S. that have the potential to host an HLW repository.

The original National Academy of Sciences recommendations (NAS 1957) proposed salt as a geologic medium favorable to hosting a nuclear waste repository. The history of U.S. policy and the approach to repository siting and development following the NAS recommendation has been well summarized by several contributors (Carter 1987; Colglazier and Langum 1988). A well-qualified site for radioactive waste disposal offers appropriate depth, formation thickness and areal extent, tectonic stability, and favorable hydrologic conditions. These criteria, demonstrated for multiple salt sites, also pertain to clay/shale formations in the U.S., as considered in this report. Clay/shale media exhibit strong positive attributes for permanent waste isolation including uniformly low hydraulic conductivity, low diffusion coefficients, and good retention capacity for radionuclides (e.g., Blümling et al. 2007). In 1979 the Interagency Review Group (IRG) for nuclear waste management, formed by President Carter, completed its report on radioactive waste management and disposal. This group concurred with the suitability of salt as a host formation, but the IRG further recommended that the federal government consider a number of sites in a variety of geologic media and select at least two, preferably in different regions of the U.S.

Consistent with the IRG recommendation, in 1982 the Nuclear Waste Policy Act (NWPA) required the federal government to identify two repository sites, and established a timetable for opening the first repository. One western desert site considered attractive for a repository was the Nevada Test Site (NTS). Investigations at the NTS included granite and argillite in addition to the volcanic tuff at Yucca Mountain. A full-scale demonstration of emplacement and recovery in granite was accomplished at the Climax stock, which confirmed the general suitability of granite disposal (Patrick 1986). Limited characterization of argillite was completed in the Eleana argillite, also on the NTS (Lappin et al. 1981). Irrespective of the potential for disposal in granite or shale media, the national repository program focused on characterizing three different media (salt, basalt, and tuff). In the 1987 NWPA amendments, the U.S. Congress decided to continue characterization of only Yucca Mountain and extended the opening date to 2010. For the ensuing 21 years, the U.S. continued site investigations and eventually developed a license application for construction authorization for a Yucca Mountain repository. The license application was submitted by the U.S. Department of Energy (DOE) to the U.S. Nuclear Regulatory Commission (NRC) in June 2008 and docketed for review in September 2008. Recently, the Obama administration issued a policy that Yucca Mountain is no longer an option for consideration as the nation's civilian nuclear waste repository. Thus, other disposal pathways are being investigated, including new concepts for geologic disposal. This report contributes to this national discussion by showing that clay/shale formations are technically viable geologic settings for permanent waste isolation in the U.S.

Before the NWPA was enacted in 1982, most repository work focused on salt formations, while other media such as granite and shale were being evaluated in other countries. Although this report focuses on clay/shale formations, it should be noted that the continental U.S. has a wealth of potentially acceptable repository sites in salt, granite, shale, and volcanic geologic formations. A substantial review of shale and argillaceous formations in the U.S. was conducted (Gonzales and Johnson 1984) before the nuclear waste program was directed to characterize only Yucca Mountain. In the U.S., there are extensive regions that have clay/shale formations with the appropriate depth and areal extent (Figure 1).

To varying degrees, clay/shale formations possess the positive attributes of low permeability, plasticity, fracture sealing or healing, and high sorption capacity. Characterization of a potential repository site in clay/shale media would also need to assess homogeneity and any complicating geologic features, such as faulting and organic content. Field-scale tests conducted by international repository programs have investigated the effect of thermal loading from HLW on permeability, fracturing, and other rock characteristics. Clay and shale naturally contain significant percentages of water, which will affect the coupled hydrologic-mechanical responses to excavation, and eventually heating. The responses also include possible desiccation, alteration of pore-fluid chemistry, and mechanical weakening or creep. These specific features and processes need to be considered in concert with the geometry, thickness, depth, and stability of the repository host rock, to assess long-term containment of radionuclides. Clay, shale and other argillaceous media have persisted tens of millions to hundreds of millions of years in almost all geologic provinces in the U.S., and have mostly remained in the same state that was acquired soon after deposition (Gonzales and Johnson 1984).

Performance assessment (PA) for the repository safety case requires knowledge of the waste inventory, the generic formation properties, and a description of the concept of disposal. Brady et al. (2009) provide an estimate of the U.S. HLW and spent nuclear fuel (SNF) inventory. DOE estimates that 109,300 metric tons heavy metal (MTHM) of HLW and SNF - primarily commercial spent nuclear fuel (CSNF) from the current fleet of reactors, but also DOE-owned defense spent nuclear fuel (DSNF), and high-level waste glass (HLWG) - will need disposal in the U.S. These estimates are used here to develop a concept for disposal operations sufficient to perform a generic, scoping analysis of waste isolation performance. The remainder of this introductory section reviews the legal and regulatory framework (Section 1.1), available clay/shale formations (Section 1.2), and previous investigations of clay/shale formations in the U.S. for repository applications (Section 1.3). The remaining sections of this report describe generic technical and performance analyses for disposal of U.S. HLW and SNF in clay/shale media. For this generic analysis, we assume a mid-range set of physical and mechanical properties for shale. Section 2 outlines the technical basis for disposal in shale, including multiphysics simulations of coupled thermal-hydrologic-mechanical processes. Analysis of heat output for CSNF and HLW is presented in Section 2.3.2. Section 3 considers potential release scenarios and the framework for a performance assessment for a clay/shale repository. Section 4 describes the generic scoping performance analysis. Section 5 concludes with a summary and recommendations for future work. Note that UNF has supplanted SNF as preferred terminology, and HLW/UNF or HLW will be used equivalently in this report.

1.1 Legal and Regulatory Framework

The 1987 Amendments to the NWPA restrict consideration of geologic repositories in the United States to a single site in volcanic tuff at Yucca Mountain, Nevada. Hence, at a minimum, consideration of a HLW/UNF repository in other formations would require changes to the legal framework specified in the NWPA.

In principle, the existing U.S. Environmental Protection Agency (EPA) HLW/UNF standard and the NRC HLW/UNF regulatory framework originally promulgated in the 1980s (40 CFR 191 and 10 CFR 60, respectively), which predate the selection of Yucca Mountain, could apply to a repository at a different site, or in another geologic medium. Indeed, the EPA standard, 40 CFR 191, currently applies to the Waste Isolation Pilot Plant (WIPP), a repository for disposal of transuranic waste from defense activities, which is located in New Mexico and situated in bedded salt. In 40 CFR 191, the primary indicator of harm is the cumulative release of radionuclides, and its measure is the complementary cumulative distribution function of the cumulative release of radionuclides that cross a boundary 5 km from the site 10^4 years after disposal, normalized by (a) EPA-derived limits for specified radionuclides and (b) the mass of radionuclides placed in the repository. However, in 1995 the National Research Council of the National Academies of Science and Engineering recommended using dose as the primary indicator of harm for a Yucca Mountain repository. The International Commission on Radiation Protection (ICRP) made a similar recommendation in 1997 (ICRP 1997), and the International Atomic Energy Agency model standard (IAEA 2006) uses a dose indicator for deep geologic disposal of radioactive waste. Because of these changes, this analysis assumes dose is the primary hazard indicator for radioactive waste disposal in clay/shale.

The EPA standard, 40 CFR 197, specifically written for a repository at Yucca Mountain, specifies the indicator measure as the expected (mean) peak dose to a reasonably maximally exposed individual (RMEI) living along the predominant groundwater flow path 18 km from the site. The standard set a limit on expected peak dose of 0.15 mSV/yr before 10^4 years and 1 mSv/yr between 10^4 and 10^6 years. The latter limit is consistent with the ICRP and IAEA recommendations. These limits are assumed applicable to the repository modeled here. The characteristics of the hypothetically exposed individual are those of the RMEI defined in 40 CFR 197. These characteristics are appropriate for humans living in arid regions similar to Yucca Mountain, but may need to be reconsidered for clay/shale disposal sites in other regions. For the purpose of this analysis, the exposed individual is assumed to live directly above the repository, rather than either 5 or 18 km away from the repository. This assumption focuses the analysis on the isolation provided by the disposal formation, and avoids speculation about sitespecific aspects of geology closer to the ground surface. Note that the EPA and NRC regulations pertaining to HLW disposal place specific requirements on those PA models that are intended to demonstrate compliance with regulatory performance objectives. The generic scoping analysis presented in Section 4 of this report represents what are likely to be the major features of a compliant performance assessment, but the scoping analysis itself does not meet all the regulatory requirements for a performance assessment.

Other details of the regulatory framework, including screening criteria for potentially relevant features, events, and processes (FEPs) and guidance on inadvertent human intrusion, are assumed to be unchanged from those stated in 40 CFR 197 for disposal of radioactive waste in a generic geologic media.

1.2 Shales and Argillaceous Strata in the United States

The generic disposal geology considered in this report represents intermediate properties in the spectrum of lithologies from poorly unconsolidated clay to argillite. There are potentially significant differences in rock characteristics across this range. Distinctions will be made when necessary, but to clarify terms, this report analyzes a fine grained, lightly indurated, detrital sediment with approximately 50% clay content and low permeability.

Sedimentary rocks are classified by the predominant grain size of their constituent materials and other textural parameters such as layering, and the composition or mineralogy of the constituent grains (e.g., clay minerals, carbonates, or quartz). Clay is a term used to describe rock-forming argillaceous minerals, rock fragments rich in clay minerals, or a detrital particle of any composition smaller than a very fine silt. Fine-grained constituents include sand, silt, and clay-sized grains (in order of descending grain size) and come from weathering of rocks. The sedimentary rocks composed predominantly of the finest sediments, clay and silt, are claystone and siltstone. If both clay and silt are present and the rock has a fine laminated or fissile texture, it is called shale. Unconsolidated silt and clay sediment together make mud, and shale is made of indurated mud with fissile lamination. Mud may be unconsolidated, such as the plastic Boom clay in Belgium, which is considered a potential repository host formation. Mudstone is a lightly indurated mud having the texture and composition of shale but lacking the fine lamination or fissility. Argillite is a compact rock derived either from mudstone, claystone, or siltstone that has undergone a somewhat higher degree of induration than mudstone or shale, but is less clearly

laminated. Argillaceous rock is slightly different from argillite in that "argillaceous" describes a rock formed predominantly from clay-sized or clay mineral particles.

Many triangular or tetrahedral diagrams have been used to guide the classification of sedimentary rocks, based on mineral type or grain-size percentages (e.g., Krumbein and Sloss 1963). The above discussion is not meant to be comprehensive in this area. Technical literature abounds with similar rock classifications, and the contributors to this study are aware of the nuances. We tolerate some overlap in nomenclature here because of the considerable literature available.

Clay minerals are generally finely crystalline hydrous silicates (mainly hydrous aluminum sheet silicates) with a two- or three-layer crystalline structure in which certain constituent elements have specific geometrical coordination (tetrahedral or octahedral). They have small particle size and substantial adsorption capability for holding water or ions (Bates and Jackson 1980). Clay mineral particles have a large ratio of surface area to volume. The most common clay minerals are kaolinite, montmorillonite, illite and chlorite, each of which is actually a group of similar minerals. Clay/shale media may contain significant fractions of water-soluble salts, calcite, chemically reducing minerals such as pyrite, and organic material.

Clay-rich, fine-grained sedimentary rocks have high ion-exchange capacity and low permeability. When not indurated they exhibit plastic deformation behavior. The sediments from which these rocks are formed were deposited over wide areas. The depositional settings changed over geologic time and location, and included areas that have more or less clay, silt, or sand as percentages. Although the current study is not a siting exercise, because of the wide availability of potential host formations in the U.S., a repository site could readily be located with attributes such as those identified by Shurr (1977):

- **Depth** The specific isolation horizon should be from 300 to 900 m below surface.
- **Shale thickness** Maximum thickness of the isolation medium is desired, while a minimum thickness of 150 m is preferred.
- **Overburden thickness** Minimal thickness of overlying geologic units is preferred.
- Lithography and mineralogy The potential repository interval should be reasonably uniform clay or shale.
- **Penetrations (boreholes)** Boreholes of any kind are undesirable, particularly if they penetrate to rocks beneath the disposal horizon. It is recognized that some holes, either preexisting or bored during detailed search for isolation sites, are necessary to provide geologic information at depth.
- **Structure** The disposal zone should have nearly horizontal bedding, with no significant faulting or folding in the vicinity of the isolation site.
- **Seismicity** Preference would be given to regions known to be inactive from recorded seismicity.

- **Topography** Minimal topographic relief is desirable to limit subsurface hydraulic gradients.
- **Mineral and water resources** It is undesirable to consider a potential site near exploitable mineral or water resources, either at or below the surface.

Because high clay content is needed to ensure low permeability and plasticity, the term "argillaceous rocks" is appropriate for the general group of desirable rock types. Gonzales and Johnson (1984) used "shale" as the general term for desirable rock types; however, the more clay-rich, plastic, less indurated, and less fissile shales could be preferred for repository purposes. Similar to Shurr's (1977) recommendation, Gonzales and Johnson concluded that the most desirable host rock units should be between 300 and 900 m below ground level, at least 75 m thick, relatively homogeneous in composition, and in an area of low seismicity and favorable hydrology that is not likely to be intensively exploited for subsurface resources. Figure 1-1 is a map of the U.S. showing distribution of principal shale formations by general geologic age and region, for which broad geologic and hydrologic data are reviewed by Gonzales and Johnson (1984). Figure 1-2 shows the location and extent of the associated principal sedimentary basins and selected smaller ones.

Table 1-1 summarizes shale and argillaceous strata of the main depositional basins in the U.S. as represented on the maps in Figures 1-1 and 1-2 (Gonzales and Johnson 1984). As shown in Table 1-1, the lower 48 contiguous states have many candidate sedimentary basins containing extensive clay/shale deposits, and representing a considerable spread over geologic time. Precambrian argillites are not included since the scant information on them indicates they are more likely to be fractured, and less likely to have satisfactory plasticity, due to diagenesis.

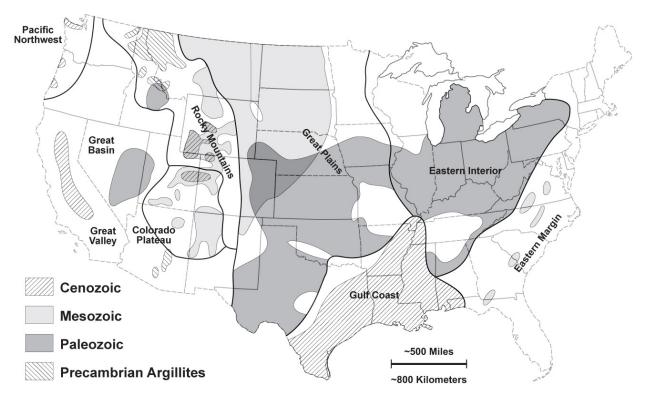


Figure 1-1. Shale Provinces in the United States (Gonzales and Johnson 1984)

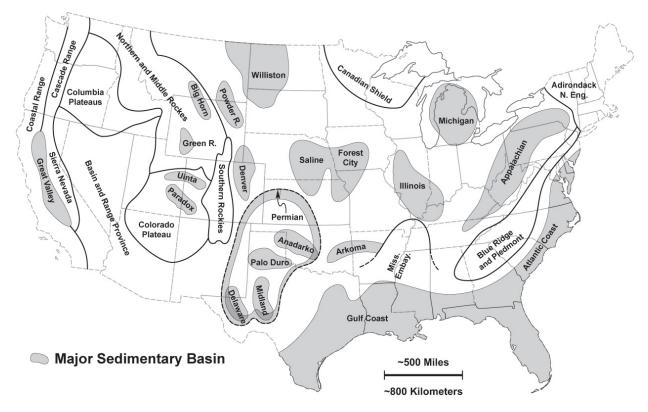


Figure 1-2. Major Sedimentary Basins in the United States (Gonzales and Johnson 1984)

Table 1-1. Shale Bodies in the United States (after Gonzales and Johnson 1984)

Location	Units	Attributes	Comments		
Eastern Interior OH, PA, NY; Appalachian, IL, and MI Basins	Six shale units in widespread areas, Paleozoic	Structurally not complex, wide basins and uplifts; seismically stable; significant petroleum and coal production in region; mostly surface water, some significant groundwater use.	Upper Ordovician shale successfully used for LPG storage, illustrating low permeability and homogeneity.		
Eastern Margin; Eastern Appalachian Mountains, Atlantic Coastal Plain	Triassic (Newark) basin, Carolina Slate belt, Cretaceous in eastern NC	Large volume of sediments with close proximity to important groundwater and not much subsurface data.	Lack of subsurface data at moderate depths, so no potentially satisfactory units are identified.		
Gulf Coast; Texas- Mexico border to FL Panhandle	Eocene Claiborne Group, TX, LA, MS, and AL	Large volume of sediments, significant clays; complex structure except in part of Mississippi Embayment; dense petroleum exploitation; significant aquifers associated with clays.	Porters Creek Clay and Yazoo Clay have good potential; some areas in LA, east TX, central AR, and northern MS without significant hydrocarbon production.		
Great Plains; west TX north to ND	Marine shales, Late Paleozoic and Cretaceous	Structurally not complex, seismically stable, many large groundwater aquifers, large petroleum exploitation basins including in shales, thickest shales (AR, OK) are petroleum reservoirs.	Pierre Shale in northern area has potential and significant areal extent; Woodford (Chattanooga) Shale (OK, KS, IA) has potential.		
Rocky Mountain Province; ID, MT, WY, UT, CO, and northern NM	Cretaceous and Tertiary	Complex structure in mountains, significant stable basins; low seismicity; most shales "soft, plastic"; significant petroleum and mineral development.	Much government land; Cretaceous shales with potential are Cody, Lewis, Steele, and Baxter Shales; Tertiary are Waltman and Green River Shales.		
Colorado Plateau; AZ, UT, CO and NM	Cretaceous and Tertiary shales	Six significant basins with thick shales, three important for petroleum.	Henry and Kaiparowits Basins (UT) may have shales with potential.		
Great Basin; NV and UT	Cambrian, Late Devonian and Mississippian	Known shales structurally complex; moderate to major seismicity; little subsurface data on shales; little information on groundwater; some mining, little petroleum.	ally Lack of data on subsurface major characteristics, so no rface potentially satisfactory units are identified.		
Great Valley of California	Cretaceous and Tertiary marine shales and clays	Moderate to major seismicity; all shales with potential are faulted and/or folded, tectonic activity continues; significant water and petroleum resources.	Shales with potential in San Joaquin and Sacramento Basins; tectonic conditions and heavy resource use may be limiting.		
Pacific Northwest; WA and OR	Tertiary	Shales faulted, folded; poor subsurface data, high seismicity.	No identified potential areas or units.		

1.3 Shale Repository Studies in the United States

In a general sense, characterization of clays or shales as possible host formations for an HLW repository in the U.S. has not been undertaken. However, from the 1970s until the mid 1980s, Oak Ridge National Laboratory (ORNL) led the U.S. research and development efforts for shale repository investigations. ORNL directed testing programs specifically to characterize a few accessible shale formations in the U.S., collecting repository-relevant physical, mechanical, mineralogical, and hydrological information. With ORNL leadership, two small-scale field tests related to repository applications were conducted by Sandia National Laboratories: (1) Eleana argillite on the Nevada Test Site (Lappin et al. 1981); and (2) Conasauga shale near Oak Ridge (Krumhansl 1983). Both of these tests were responsive to the IRG recommendations to evaluate rock types other than salt, as mentioned above.

The Eleana argillite surface heater test was launched in 1976 and ran three years. Within an area on and near the NTS, the Eleana Formation outcrops abundantly and exists in structures of sufficient size and thickness to accommodate a repository. On the NTS, the Eleana Formation totals more than 3000 m thickness. Chemical analyses of several samples showed the bulk composition of argillite for the Eleana Formation is transitional between that of representative normal shale and residual clay. Because the Eleana Formation is highly jointed, it possesses little tensile strength. In compression, however, it displays a linear stress strain response and uniaxial strength of over 40 MPa. The single-heater test was conducted in a borehole 24.4 m deep, with the 4-m heater situated near the bottom (Lappin et al. 1981).

Based on divergence of modeled and measured temperatures at high temperatures, and the apparent coupling of thermal and mechanical properties *in situ*, additional testing would be required to characterize *in situ* response. It is also notable that the test was conducted near the ground surface, where initial *in situ* stresses were negligible. Creep, which could be important at depth, was therefore not evaluated. The heating response of Eleana argillite involved volumetric contraction of the rock at the test depth, which would likely be different if tested below the water table. Post-test gas transmissivity testing indicated that formation permeability within a radius of 1.2 m increased by roughly three orders of magnitude.

The Eleana near-surface heater experiment did not qualify either argillaceous rock or argillite specifically as repository media, nor was it intended to do so. However, the experiment did not reveal any mechanism that would eliminate argillaceous rocks from consideration for a HLW repository (Lappin et al. 1981).

The Conasauga Formation test was situated in a friable, silty, illitic shale that is interstratified with numerous layers of limestone and siltstone. Unlike the test in Eleana shale, groundwater was constantly available to refill the network of fine fractures present in the shallow subsurface. Thermal reflux of water was apparently continuous, resulting in the precipitation of a shale-anhydrite boot around the base of one heater. In the case of the Conasauga tests, the *in situ* rock mass modulus may have been so small that the rock mass collapsed, even at near-surface stress levels. In addition to the possibility of collapse, mineralogical reactions in the Conasauga tests may have precipitated new phases in existing joints, thereby decreasing the permeability. Krumhansl (1983) concluded that the thermal and mechanical data obtained from this experiment reflect favorably on shale as a medium for HLW disposal.

As suggested by these test descriptions, testing efforts to characterize thermomechanical responses of shale formations in the U.S. were rudimentary. More field work would be needed to characterize any particular clay/shale site, and this should include development of an underground research laboratory (URL). There currently are no plans for the U.S. waste program to advance to the stage of URL development in a clay/shale formation, so international collaboration may be a key source of information as the U.S. contemplates alternative disposal pathways.

As noted, clay/shale formations that could host a repository for HLW/UNF in the U.S. span a range of lithologies, with different physical, mechanical, hydrological, chemical, and mineralogical properties. Two primary concerns for evaluating the effects of repository construction and operation on long-term waste isolation performance are geomechanical response and fluid flow. The specific properties that control these effects would be among those that are closely examined at the time of site selection and characterization. Clay/shale properties are reviewed in the following section, presenting shale repository design considerations, and in Section 2.3.2, which introduces the importance of coupled processes.

1.4 Representative Shale Information

This section develops a generic clay repository concept that is applicable for a range of possible rock characteristics. The host formation is considered to have very low undisturbed permeability at all scales important to repository performance. If the formation exhibits a brittle style of deformation in laboratory and field-scale tests, then advective fluid flow may occur in fractures induced by excavation or heating. If the host material is plastic, fracture flow is less important because fractures tend to seal or heal, and diffusion becomes the dominant transport process. The same repository concept (layout, packaging, etc.) could be applied to both types of lithology.

An exhaustive study by the "Clay Club" (OECD NEA 1996) describes the basic physical and chemical processes that combine to control the flow of water, gas, and solute through argillaceous media. Much is known about these processes, but without a specific site in mind our study selects from a range of properties encountered in clay/shale repository studies reported internationally. We project that these selections are reasonably representative of potential host rocks in the U.S.

To choose representative material properties for our analyses, we turn to international programs that have characterized several clay formations. These include:

- Opalinus claystone at Mont Terri, Switzerland
- Callovo-Oxfordian argillite/mudstone near Bure, in eastern France
- Boom clay at Mol, Belgium.

Opalinus clay is a bedded, stiff, Mesozoic claystone of marine origin. The Opalinus formation is composed of 50% to 65% clay (Table 1-2) and has a low water content (4% to 6%). Most of the clay is kaolinite and illite. Like most argillaceous rocks, the laboratory-measured properties are transversely isotropic (Corkum and Martin 2007b). Typical of many geomaterials, the response to deformation is generally brittle. This is in agreement with extensional fractures observed around underground excavations in the Mont Terri URL, particularly in zones of high deviatoric

stresses where the shear mode of yielding might be anticipated (Martin and Lanyon 2003). The Opalinus clay is an indurated claystone with reasonable engineering strength properties, including a comparatively high cohesive component of shear strength, of 2.2 and 5 MPa parallel and perpendicular to bedding, respectively. Strength of the Opalinus clay is sufficient to allow small, unlined tunnels and larger, lined tunnels to be constructed at depths of several hundred meters. When subjected to heating, saturated stiff claystone exhibits a strong pore pressure response that affects the hydraulic and mechanical behavior of the material (Gens et al. 2007).

Callovo-Oxfordian argillites were deposited approximately 155 million years ago. They have a total thickness of approximately 130 m at the URL site. Reported average compositions vary in the stratigraphic sequence, with respect to percentages of carbonate (23%), clay (55%), and quartz and feldspars (20%) (ANDRA 2005). The Callovo-Oxfordian argillites are comparable to the Opalinus clay from Mont Terri: both are chemically reducing media with low permeability and small pore size. Transport is diffusion dominated, and both lithologies have more than sufficient compressive strength for repository applications (Table 1-2).

Boom clay mineralogical analyses show a wide variation in the content of clay minerals (30% to 70%, with an average of 55%), which reflects stratigraphic heterogeneity. These clay minerals are complemented by quartz, feldspars, carbonates, pyrite, and organic matter. The porosity of the Boom clay, and hence its water content, is approximately 20% to 30% by volume (Table 1-2). Geophysical borehole logs show that these properties are fairly constant throughout the Boom clay thickness, except for zones at the bottom of the unit and at the top of the upper transition zone.

As noted in Section 1.3, two heater tests were performed in U.S. shale formations for preliminary characterization of mesoscale thermal-hydrologic-mechanical behavior, with a view to repository applications. These testing programs were ended before ancillary laboratory testing was completed to quantify other properties needed for repository assessment. Accordingly, we look to international programs and their advanced repository work for the fundamental characteristics of potential clay/shale repository rocks. One shale formation in North America, Pierre Shale, was characterized sufficiently that its properties could be compared to the three European sites, in the "Clay Club" report (OECD NEA 1996).

Table 1-2 summarizes some of the most pertinent properties for three well-characterized clay formations from the international repository programs. All characteristics except geologic age and organic content are given in the NEA catalogue (Boisson 2005). In addition to the name and location, we list classification, predominant mineralogy, hydraulic conductivity, and strength. Table 1-2 supports the point made previously that the European programs, which have advanced repository sciences in clay/shale media, represent a wide range of rock characteristics. As will be shown in Section 4, the most important formation characteristics with respect to long term performance are low hydraulic conductivity and high sorption properties. Generally satisfactory depth, thickness, and usable area are highly desirable and allow boundary conditions to be established for this analysis. To a certain extent, engineering can mitigate operational difficulties associated with weaker rock types, so strength properties are not critical to this assessment.

To summarize, the United States has an abundance of potential HLW repository host formations, be they salt, granite, clay, shale, or volcanic. A shale repository program was underway during the 1970s and 1980s before national policy directed the program elsewhere. Shale repository studies culminated with a workshop in 1985 (ORNL 1986). Since that time, European repository programs have continued to advance clay/shale repository concepts and provide tangible assurance and confidence that a repository can be built and operated to permanently isolate HLW.

Table 1-2. Approximate Properties of Well-Characterized Clay Formations

Shale Formation	Reference Location	Approximate Geologic Age (Ma)	Typical Thickness (m)	Top Burial Depth Present/Past (m)	Clay Content (wt. %)	Classification ¹	Mineralogy ²	Carbonate Content (wt. %)	Hydraulic Conductivity (m/sec)	Compressive Strength ³ (MPa)	Organic Content (wt. %)	In situ Water Content (vol. %)
Europe:	Europe:											
Opalinus Clay	Mont Terri, CH	180	160	250/1350	50 to 65	Claystone	Kaolinite, illite, illite, illite/smectite	10 to 50	Est. 5×10^{-13} to 6×10^{-14}	12	0.5	4 to 6
Callovo- Oxfordian Argillite	Bure, France	155	130	400/na	45	Mudstone	Illite/smectite	20 to 30	Est. 3 × 10 ⁻¹⁴	25	< 3	5 to 8
Boom Clay	Mol, Belgium	30	100	220/na	55	Bedded mud	Smectite/illite	1 to 5	Est. 6 × 10 ⁻¹²	2	1 to 5	22 to 27
North America (example formation included in OECD/NEA 1996 tabulation):												
Pierre Shale	Pierre, SD	70	400	150/na	50	Mudstone	Illite/smectite	0 to 50	10 ⁻¹³ to 10 ^{-14.6}	7	0.5 to 13	~16 (variable)

Sources: ANDRA 2005; Hansen and Vogt 1987; NAGRA 2002; NEA 2003; Neuzil 2000; Volckaert et al. 2005.

¹ Use clay-mud-claystone-mudstone-argillite classification from OECD/NEA 1996, p. 4. ² Predominant assemblage or combination: smectite, illite, kaolinite, chlorite, carbonate, etc. ³ Unconfined, typical laboratory values for fresh samples.

NOTE: na = not applicable.

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2. TECHNICAL BASIS AND CHARACTERIZATION

Disposal of HLW/UNF in a clay/shale formation is expected to provide effective long-term (> 1 million years) isolation of radionuclides from the biosphere because of the following hydrologic, chemical, and mechanical characteristics:

- **Slow fluid movement** Fluid movement in clay or shale is slow because of very low hydraulic conductivity (typically 10^{-12} m/sec or less). Application of advective-diffusive transport modeling (described in Sections 2.4.5 and 4) shows that diffusion is the primary transport mechanism for 1,000,000 years, after the thermal pulse.
- Self-sealing The shale type selected for this generic analysis is ductile, so that fractures formed by excavation and heating will close and seal during repository operation and during the first few hundred years after closure. Fluid movement through repository access tunnel and shaft seals will likewise be limited by the low permeability of candidate seal materials (Section 2.1.3). Low permeability and self-sealing of fractures around openings are primary favorable features of clay/shale media.
- Chemical conditions limit radionuclide release and transport Reducing conditions will prevail within the repository and the host unit, which will maintain waste forms and most radionuclides at very low solubilities. Sorption of many radionuclides onto clays with high specific surface area will also retard transport.

The clay/shale repository concept is developed here in view of conceptual designs advanced by the Belgian, French, and Swiss programs. To establish the boundary conditions for analysis we specify:

- Waste inventory and description We assume permanent disposal for the inventory described in Appendix A (Brady et al. 2009) for the generic performance analysis. We recognize the tenets of retrievability and reversibility inasmuch as they have been incorporated into international repository programs. However, geologic disposal should permanently isolate waste material from the biosphere and not be predicated on retrievability. Therefore, for the purpose of this study, retrievability is not a design priority, although reversibility and retrieval are not precluded for the generic design concept adopted.
- **Geologic setting** A repository would be deep enough below the present land surface to ensure that the waste is not exposed to the biosphere through erosion or denudation during its hazardous period. To address the slow removal of the land surface through erosion, which generally is proceeding at an average rate of 2.5 to 7.5 m per 100,000 years in the continental United States (Ritter 1967), and to avoid the shallow circulation of fresh groundwater that might contact the upper parts of the host rock formation, the repository would be situated at least 300 m beneath the present land surface. Although groundwater aquifers may overlie the host formation, the site would be selected to minimize the likelihood for future exploitation of groundwater or other resources in strata below the host formation.

• **Concept of operations** – Based on disposal concepts in Europe, disposal operations for this generic repository would be horizontal. The operational choice between vertical and horizontal handling and placement of waste canisters greatly influences repository design. The French program opted for horizontal placement because vertical handling would require additional overhead space, and horizontal waste handling allows more compact design. The repository would be accessed by vertical shafts.

To select design information and clay/shale properties for this analysis, comparison is made with the advanced international repository programs that are focused on clay/shale media. There is a vast amount of descriptive information available. From international experience, some of the basic parametric selections for this generic study are: horizontal emplacement layout, geometries for emplacement and access openings, and host rock properties. Our proposed sealing system has been well developed and previously certified, as discussed below. Given a selection of host rock characteristics, waste inventory, and concept of operation, the appropriate FEPs are identified in Section 3.1, for the generic safety analysis.

As discussed in Section 1.1, we expect that the overall repository waste isolation performance measure of interest would be mean annual dose to a hypothetical individual, with limits set at 0.15 mSv/yr for 10,000 years following disposal, and 1 mSv/yr for the period between 10,000 years and 1 million years. Other details of the regulatory framework, including screening criteria for potentially relevant FEPs, are assumed to be unchanged from those stated in 40 CFR Part 197 and 10 CFR Part 63.

To support the multi-physics modeling described in Section 2.4 and the performance analysis of Section 4, an underlying technical basis is selected for the physical design, the predicted thermal effects, and the near-field chemical characteristics. Section 2.1 describes a modular repository design for clay/shale media. Section 2.2 describes seals. Section 2.3 describes the thermal effects from decay heat on the host clay/shale formation, and the temperatures expected considering the range of thermal loading possible with currently available UNF and HLWG waste forms. Section 2.4 presents multi-physics numerical simulations of coupled responses to excavation and heating, for thermally bounding conditions, and for a typical "young" HLWG waste form. Section 2.5 outlines the chemical characteristics of the repository.

2.1 Shale Repository Design

Three basic components govern repository design: waste inventory, geologic setting, and a concept of operations. The canister size and heat generation will strongly influence the actual design, including the extent of the underground facility and the minimum vertical thickness of the host formation. The geochemical environment expected in emplacement boreholes will also influence the design, including backfill if necessary, and seal systems. Each of these specific topics is covered in the following sections of this report.

Because France has an advanced concept for a repository in the Callovo-Oxfordian argillite, and a reasonably clear nuclear future, their experience will be used to inform our generic repository design. The French radioactive waste program is investigating an argillite formation in a 200 km² region in eastern France. The candidate rock unit is 130 m thick, centered at 500 m depth. The formation exhibits the following characteristics important to the safety case: homogeneity,

limited fracturing, low permeability, reducing environment, emplacement areas with no evidence for preferential flow paths, and favorable geochemistry. The French program has analyzed the host rock responses to excavation, desaturation-resaturation, dessication by ventilation, heating, chemical interaction with concrete, and hydrogen production by corrosion reactions. The only potentially significant, direct interaction of the repository with surrounding formations would occur via advective flowpaths associated with access shafts or ramps (ANDRA 2005).

The mechanical properties of the Callovo-Oxfordian argillite require ground support to ensure operational safety during construction, waste emplacement, and possible waste retrieval. The overall inventory includes long-lived intermediate-level waste and vitrified HLW. The vitrified waste is characterized by high heat production. Recognizing that the type and quantity of waste would influence repository design, our generic assessment considers mainly heat-generating waste. We extract guidance from the considerations given by the French to disposal of thermally hot, vitrified HLW, and recognize the existing waste inventory in the U.S. (Appendix A). Heat generation of vitrified HLW will drive evolution of near-field rock characteristics. Guidelines for ANDRA currently attribute a water tightness function to the disposal packages for vitrified HLW. ANDRA retrieval obligations rely heavily on waste package integrity. The French repository design ensures that peak temperatures will not exceed 100°C anywhere, and will generally be 80°C or lower. The French concept for a repository is modular, with each module comprising one or more disposal cells along with the drifts to access them. A disposal cell is the horizontal borehole in which disposal packages are placed.

Many design variations are possible, but because this is a generic analysis and not a design, we borrow ideas from advanced clay/shale programs for analysis purposes. The repository footprint would depend on the concept of operations and the waste form characteristics, which in turn depend on the duration of surface storage prior to emplacement in the repository. For example, the French design maintains a distance between two adjacent disposal boreholes of at least five times their diameter. This basic design layout aids mechanical stability and thermal management. The geometric configuration of the French underground installations and the thermal management of the HLW are designed to limit the temperature to 90°C in contact with the rock or buffer. The layout of repository zones for HLW and UNF disposal will depend on the waste inventory and thermal decay characteristics.

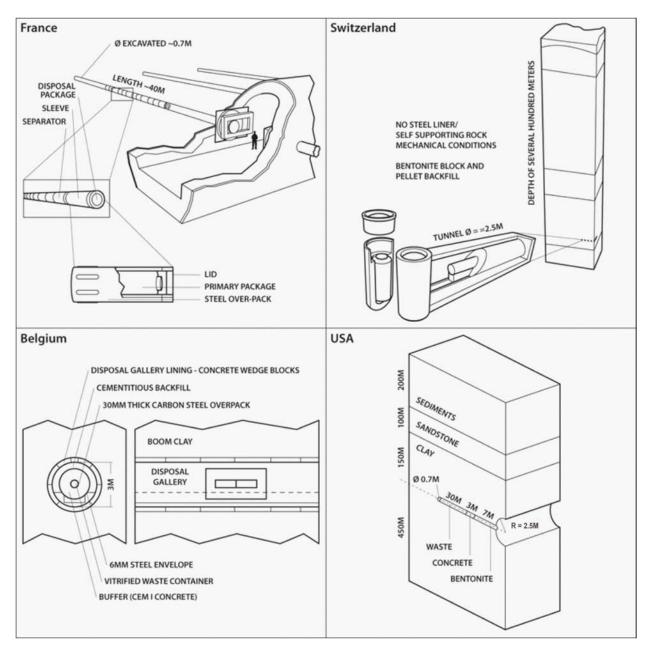
In Switzerland, NAGRA is studying the feasibility of an underground repository in claystone formation (Opalinus clay) with mineralogical characteristics similar to that of the argillite at the Bure site. The NAGRA concept will install waste canisters in emplacement tunnels, which will then be backfilled. The HLW/UNF canisters will be placed on highly compacted bentonite clay blocks, co-axially with the tunnel axis, with a distance of 3 m between canisters. No steel liner is currently designed for the horizontal disposal concept because of favorable rock mechanical properties. The clay buffer material used to backfill the tunnels will act as an extra measure of compartmentalization and isolation of the waste canisters. Retrievability is believed possible, but is not the highest priority design requirement.

In Belgium, the repository concept is adapted to a geologic formation with less mechanical strength (see Table 1-2). The ONDRAF concept includes horizontal disposal and a "supercontainer" concept. Owing to the low strength of the Boom clay, the disposal galleries will be structurally supported by a liner built from circumferential concrete wedge blocks. The

vitrified HLW will first be encapsulated in a 2-m diameter package, which will then be placed in 3.6-m diameter openings at the disposal horizon. The entire annulus will eventually be filled with cementitious backfill. The supercontainer constructed in this manner is expected to remain intact throughout the thermal pulse.

Our generic repository design concept borrows strongly from the experience and expertise of these existing shale repository programs. Figure 2.1-1 illustrates sketches of the intended disposal process for the three comparable European repository studies, and a representation of possible disposal in a clay/shale formation in the U.S. We have opted for horizontal placement in an unlined and unbackfilled borehole, 0.7 m in diameter and 40 m in length. The disposal borehole will be sealed at the proximal end with concrete and bentonite as depicted in Figure 2.1-1 (USA). Our disposal boreholes would be spaced far enough apart to limit interaction of neighboring boreholes (Section 2.3.2 evaluates the spacing between emplacement boreholes, which would be needed to accommodate the range of waste forms currently available in the U.S.). The access drifts are conceived to be 5 m in diameter, which can accommodate waste packages containing UNF assemblies or HLWG, but could be expanded to allow additional room for construction and waste handling equipment. These features and dimensions are generally consistent with the French layout shown in Figure 2.1-1 (France), but could be changed in response to site specific analyses. Structural analysis of this disposal concept is presented in Section 2.4. Further technical details are provided in the following sections, which describe the performance of a clay/shale repository for HLW and UNF.

International program comparison studies performed to date (NWTRB 2009) have concluded that the long-term performance of an engineered barrier system is unimportant to the safety case, for disposal in clay/shale media. The Belgian approach envisions an engineered barrier consisting of stainless steel canisters holding HLW inside a carbon steel overpack surrounded by thick concrete. The French engineered barrier consists of vitrified waste placed within stainless steel packages. The Swiss engineered barrier concept envisions cast iron canisters for HLW and commercial SNF. HLW will be contained in a stainless steel flask inside the canister. The iron canisters will be surrounded by bentonite clay. Thus, the waste package, though integral to the disposal operational concept, can readily be engineered to meet design or manufacturing objectives.



Sources: France: <u>www.andra.fr;</u> Switzerland: <u>www.nagra.ch;</u> Belgium: <u>www.sckcen.be</u>. Figure 2.1-1. Schematic of Clay/Shale Disposal Concepts

2.2 Seals

The fundamental design principle for seal systems in a clay/shale repository is to ensure that radionuclide transport is controlled by diffusive rather than advective processes. Access tunnel and shaft seals have a hydraulic function to limit water flow from disposal cells to access shafts or ramps, to zero or specified acceptable levels. Given the time scale for natural resaturation of swelling clay seal materials, corresponding activities must be developed to provide evidence that seals will function as designed, without having to monitor the seals in their long-term configurations. Fortunately, extensive design, analysis, and testing for shaft seals were performed for the WIPP repository, which provides the basis for performance expectations in this generic study. The design of the seal system for a shale repository would benefit from design and performance calculations on seal systems developed for the WIPP, which were subject to extensive technical peer review and comprise published portions of the Compliance Certification Application to the Environmental Protection Agency.

An acceptable seal system can be designed and constructed using existing technology, and the seal system can readily meet requirements associated with repository system performance. These goals were met for WIPP by using a set of guidelines that incorporates seal performance issues, and with a commitment that the seal system design would implement accepted engineering principles and practices. These guidelines were formalized as design guidance for the shaft seal system:

- Limit waste constituents reaching regulatory boundaries
- Restrict formation water flow through the sealing system
- Use materials possessing mechanical and chemical compatibility
- Protect against structural failure of system components
- Limit subsidence and prevent accidental entry
- Utilize available construction methods and materials.

The WIPP experience established that effective seal systems can be designed, tested, analyzed and subsequently installed. The design approach applies redundancy to functional elements and specifies multiple, common, low-permeability materials to ensure reliable performance. The system described below uses engineered materials with high density and low permeability to completely fill the shafts. Laboratory and field measurements of component properties and performance provide the basis for the design and related evaluations. Hydrologic, mechanical, thermal, and physical features of the system were evaluated in a series of calculations, which show that the design effectively limits transport of fluids within the shafts, thereby limiting transport of waste material to regulatory boundaries. Additionally, the use or adaptation of existing technologies for seal construction combined with the use of available common materials assures that the design can be constructed.

Repository seal systems would be critical to the success of a repository in clay/shale media. The sequence of repository operations would include construction, waste emplacement, installation of seals, repository closure, and abandonment. However, owing to the potentially long time periods involved, considerations such as loss of institutional control enter into the design and concept of operations. Events such as war or natural disaster may lead to premature repository abandonment. These hypothetical futures have been considered by many, if not all, repository

programs. The impact of these unlikely situations is minimized by sealing emplacement drifts in modular compartments in due course of disposal operations. The French concept, as an example, closes the repository in stages, i.e., disposal cell sealing, backfilling, and sealing drifts and then shafts. Seal materials include concrete and swelling clay, consistent with WIPP shaft seal material specifications.

The shaft seal system would limit entry of formation water into the repository and restrict the release of fluids that might carry contaminants. Seals are designed to limit fluid transport through the opening itself, along the interface between the seal material and the host rock, and within the disturbed rock surrounding the opening. The shaft seal system design for WIPP was completed under a quality assurance program that meets EPA regulations including review by independent, qualified experts to assure the best possible information is provided. Technical reviewers examined the complete design including conceptual, mathematical, and numerical models and computer codes. The design reduces the impact of uncertainty associated with any particular element by using multiple sealing system components and by using components constructed from different materials. The seal system applied to a clay/shale repository would include a modular concept whereby the whole repository comprises sections or modules that are sequentially partitioned and isolated with horizontal panel closures (seals). The repository modules would be separated from one another by sufficient distance that thermal, hydrologic, and other possible modes of interference are inconsequential. After the repository is filled with emplaced waste and horizontal panels are closed, seals would be installed in the access shafts.

The potential geologic and hydrologic settings (Sections 2.3, 2.4, and 3.1) can combine to provide excellent waste isolation performance as the repository would resaturate, and the host rock would deform plastically, ultimately sealing the excavated openings. The disposal horizon is assumed to be at a depth of 450 m, although depths from 200 to 600 m would be acceptable. From the disposal horizon upward the shaft seal system would include the following components:

- Shaft Station Monolith The base of the shaft will be sealed with Portland cement based concrete. It will be placed by tremie line techniques against non-removable (committed material) forms, which could be fabricated from concrete block or other abutments.
- Clay Columns A sodium bentonite compacted clay component is placed on top of the mass of concrete. Alternative construction methods including block placement and dynamic compaction are viable. Clay columns effectively limit formation water movement from the time they are placed. The swelling pressure associated with the clay column is sufficient to promote sealing of fractures in the surrounding rock near the bottom of the shafts, thus removing the proximal excavation damage zone (EDZ) as a potential pathway.
- Asphalt Column Asphalt is a widely used construction material with properties considered desirable for sealing applications. Asphalt is readily adhesive, highly waterproof, and durable. Furthermore, it is a plastic substance that provides controlled flexibility to mixtures of mineral aggregates with which it is usually combined. It is highly resistant to most acids, salts, and alkalis. A number of asphalts and asphalt mixes

are available that cover a wide range of viscoelastic properties and which can be tailored to design requirements.

• Earthen Fill – The upper shaft is filled with locally available earthen fill. Most of the fill is dynamically compacted (for example, using the same method used to construct the compacted clay column) to a density approximating the surrounding lithologies. The uppermost earthen fill is compacted with a sheeps-foot roller or vibratory plate compactor.

For sealing a repository in a clay/shale formation, the engineering and material specifications developed for the WIPP can be translated with minor modification of functional and operational requirements. Notably, the salt component of the WIPP shaft seal system would not be installed. Otherwise, the seal material specifications, construction methods, rock mechanical analyses, and fluid flow evaluations developed for the WIPP remain applicable. This design concept is not the only possible combination of materials and construction strategies that would adequately limit fluid flow within the shafts.

A major intrinsic advantage of repository development in a clay/shale formation is an overall lack of groundwater to seal against. Even though regional aquifers may be proximal to the host clay/shale unit, the shaft seal system would be designed to perform in contact with groundwater. If water flow occurs within the repository openings or in the EDZ, the chemistry of water or brine could impact engineered materials. However, the geochemical setting will have little influence on the concrete, asphalt, and clay shaft seal materials. Each material is durable with minimal potential for degradation or alteration. Note that microbial degradation, material interactions, and mineral transformations are often incompletely understood, and therefore are the focus of ongoing research. Degradation of concrete is possible, but unlikely as only small volumes of groundwater will ever reach the concrete. Moreover, in a closed system, such as the hydrologic setting for these shafts, cement phase transformations would decrease the permeability of concrete seal elements.

Asphalt used as a seal component deep in the shaft will occupy a benign environment, with no ultraviolet light or oxidizing atmosphere that could degrade its sealing capability. Additional assurance against possible microbial degradation in asphalt elements used in the shaft seal design could be provided with addition of lime. For these reasons, it is believed that asphalt components can retain their design characteristics for an indefinitely long period.

Natural bentonite is a widely used, geologically stable sealing material. Three internal mechanisms, illitization, silicification, and ion exchange, could affect sealing properties of bentonite. Illitization and silicification are thermally driven processes unlikely to occur in the shale environment over the period of regulatory concern. Significant degradation due to ion exchange would require extensive fluid transport of Ca through the bentonite and Na away from the seal, which is unlikely. Wyoming bentonite – the specified material for the seal system – has existed unaltered for well over a million years in its natural environment.

The shaft seal system described above could be constructed using off-the-shelf technology. A more comprehensive treatment and specific analyses are available in Hansen and Knowles (2000). The seal design system for a clay/shale repository would very likely be modified,

perhaps simplified, and construction alternatives may be implemented during repository development. This section establishes a frame of reference for shaft seal design and analysis for a potential clay/shale repository for HLW in the U.S.

2.3 Thermal-Hydrologic-Mechanical Conditions in the Host Rock

Clay/shale formations have naturally low permeability and self-sealing characteristics favorable to waste isolation. This section describes the range of clay characteristics investigated by European waste disposal research and development (R&D) programs, and how those characteristics are likely to change as a result of underground excavation and construction, waste emplacement, and heat generation. These considerations lead to a preferred approach for representing hydrologic and geochemical conditions for radionuclide transport in the generic performance analysis.

The clay/shale formations available for geologic disposal applications in the U.S. were deposited in marine or lacustrine environments. They were typically deposited as porous muds, with high water content but low permeability, which became indurated over time by continued deposition and burial, compaction, and varying degrees of diagenesis. The indurated sediments being investigated by the Swiss and French repository programs (the Opalinus claystone and the Callovo-Oxfordian mudstone) are considered typical of available media for this assessment.

2.3.1 Excavation/Construction Effects

One of the most widely discussed aspects of repository host rock regardless of lithology is the damage caused by excavation. A repository rock that has the capacity to re-seal or heal fractures in the EDZ would be highly desirable for isolation purposes. The possibility of healing microfractures in salt under conditions at WIPP, for example, has been well established (Hansen 2003). Creation, evolution, healing and/or mitigation of the EDZ are of significant importance to seal system design and assessments of long-term safety. Blümling et al. (2007) reviewed comprehensive investigations at different sites (e.g., HADES, Belgium; Mont Terri, Switzerland; Tournemire, France) and showed that an EDZ occurs in soft or plastic clays as well as in indurated and more brittle claystones or argillites. The character of the EDZ is considered here for a generic clay repository for HLW in the U.S. As discussed below, the impact of tunnel convergence and self-sealing on the long-term hydraulic properties of the EDZ has not yet been examined at full scale. However, based on process understanding and coupled process modeling results, the EDZ is expected to have a thickness of 2 m or less, and the long-term effective hydraulic conductivity of the EDZ in clay/shale host rock is expected to be increased by approximately one order of magnitude or less, relative to the undisturbed rock (NAGRA 2002).

The EDZ for any excavation is created by changes to the preexisting stress state and is a function of the material properties in relation to the stress conditions. Fractures have an appreciable effect on the permeability of the host rock and therefore their extent and characteristics are important to quantify. In addition for clay/shale media, the EDZ is also influenced by near-field desaturation and dessication that may lead to local fracturing and material weakening. In most rock types, the extent and shape of the EDZ can be measured and calculated.

Evolution of the EDZ in salt is very sensitive to the stress state and exhibits steep transient deformation behavior that evolves into steady-state deformation. This behavior is well understood in terms of plastic dislocation mechanisms in salt crystals. Hence, creep closure of underground openings in salt at ambient temperature is understood at a mechanistic level. By virtue of several studies at WIPP, the nature of the EDZ can be adequately described for engineering and analysis purposes in terms of stress invariants, which is conducive to finite element calculations (Hansen 2003). Long-term behavior including healing can be assessed by tracking the stress state within the structural calculation. This approach, which has proven utility in salt, is assumed to be applicable in the generic clay repository evaluated here.

Indurated clay formations have bedded structure that causes them to respond as anisotropic, cohesive materials (Blümling et al. 2007). An EDZ with increased permeability forms around openings in all types of clay rocks from the effects of excavation and construction. The following conceptual description of the EDZ in indurated clay/shale rock types is based on investigations performed in European underground laboratories. We also summarize how the EDZ has been represented in preliminary performance assessments for repositories situated in these clay formations.

Performance assessment for clay repositories must consider whether increased permeability in the EDZ could support a pathway for radionuclide transport either to the radial limit of the zone, or along the EDZ parallel to the excavated openings. The undisturbed permeability of clay formations is so small that liquid-phase advective transport in the far field is negligible (Section 2.3.3). Such low permeability results from the impermeable nature of clay in general, and also a lack of permeable fractures open to flow. Fractures have been observed in quarry or pit excavations of clay/shale formations being investigated in Europe (Arnould 2006), where fracture spacings from a few mm to 1 m are observed in surface exposures (where stress release and weathering have occurred). However, these are closed by confining pressure at depth and are not generally observed. Such fractures have apparently never before been open, and have never conducted significant fluid flow, because they are not locally altered by exposure to water and have no filling mineral deposits. Hence, although fractures may be formed and/or opened by stress changes and deformation in the EDZ, if no alteration occurs they can subsequently close, re-establishing low permeability.

Excavation in many geologic media causes mechanical damage to the rock around the opening, which forms and immediately stabilizes during excavation. As the excavation advances, and the *in situ* stress is redistributed away from the opening, the stress state of the adjacent rock becomes increasingly deviatoric and less confined. The resulting deformation determines the nature and extent of the EDZ. In clay/shale media this immediate response has been modeled using elastoplastic constitutive equations, and other approaches (Corkum and Martin 2007a; Gens et al. 2007). The immediate response is followed by time-dependent pore pressure effects (lasting days or weeks), mechanical creep (lasting years), and response to thermal loading, as discussed below.

The initial extent of the EDZ around openings in clay/shale formations is determined by rock strength and deformation properties, initial liquid saturation, *in situ* stress conditions, the opening size, and the resulting pore pressure changes. These processes will produce micro- and macro-scale fractures that increase permeability (NAGRA 2002). The increased permeability will eventually be reversed, at least in part, by sealing processes which include swelling,

disintegration, creep, and consolidation (Bernier et al. 2007). The initial rock hydraulic conductivity (Table 1-2) of the EDZ near the openings for a repository in clay/shale would be increased by orders of magnitude compared to the initial undisturbed conductivity, to as much as 10^{-8} m/sec, followed by reduction due to sealing over the next few years. Sealing of fractures and other voids that form during excavation will cause the final hydraulic conductivity of the EDZ to be less than 10^{-12} m/sec after a few years, especially if the opening is backfilled with a swelling material such as bentonite (considering the Opalinus clay to be representative; Blümling et al. 2007).

The availability of moisture is important because clay/shale media have affinity for moisture, which causes softening and strength reduction (Gens et al. 2007; Boisson 2005), and swelling (1% to 7% swelling capacity; NAGRA 2002). Conversely, partial desaturation is likely to occur by evaporation during ventilation for a few years during the operational phase of a repository, and cause shrinkage and stiffening of the clay, and resistance to creep (ANDRA 2005). Cyclic drying and rewetting may be reversible, but can cause textural changes and disintegration of the material around the opening. After the emplacement openings (horizontal boreholes) are closed, resaturation will occur gradually, accompanied by swelling and creep. Eventually, the emplacement openings will close, and buffer material used in the installation, if any, will be hydrated.

Hydro-Mechanical (HM) Coupling – A time-dependent pore pressure response to excavation occurs in clay rocks because these media have very low permeability and high initial water saturation. Local changes in normal stress caused by excavation produce changes in pore pressure, and the low permeability inhibits drainage. The locally increased pore pressure decreases the effective stress acting through the solid framework, and causes dilation in directions transverse to loading. Pore water may drain in response to increased pressure, increasing the deviatoric stress. These changes, combined with stress redistribution near excavated openings, locally reduce the rock strength and produce additional deformation. Coupled hydro-mechanical models for excavation response of indurated clay/shale media have combined pore pressure effects with excavation response by elasto-plasticity (e.g., Uhlig et al. 2007) and damage-state models (e.g., Gens et al. 2007).

The strength and deformability of clay/shale rocks are thus related to water content. The effect differs from the effective stress principle in permeable media with connected pore space, because of the strong particle interactions (disjoining pressure) and low permeability. In clay-rich rocks, excavation-induced pore pressure changes dissipate over days or weeks, as observed in a field-scale experiment in the Opalinus formation (Gens et al. 2007). During this period of drainage, the spatial extent of potential damage increases as the region of elevated pore pressure expands. Near the opening, the magnitude of the volume strain and thus the potential for damage is greatest due to dilation, activation of planes of weakness, and creep. The relationship between volume strain and hydraulic conductivity is uncertain, but variability in porosity has been related to hydraulic conductivity in various clay media (Boisson 2005).

Overconsolidation of clay/shale formations occurs when *in situ* loading conditions in the history of a deposit have exceeded the present loading conditions. For example, overconsolidation occurs when a soft shale formation is subjected to deep burial, then uplift and erosion of overburden. The rock retains the compaction and deformation properties associated with

maximum burial, potentially for millions of years. Overconsolidation leads to compaction of the solid framework, reduced porosity and water content, increased stiffness and elasticity, and may cause increased dilatancy in response to deviatoric stress conditions (Prashant and Penumadu 2004). Overconsolidation affects the constitutive behavior used to model rock response to excavation, and may also affect response to heating. Increased dilatancy is important because it has the potential to increase porosity and permeability in the repository near-field host rock. Overconsolidation and its effects on repository-relevant rock characteristics are the subject of active investigations in the laboratory and *in situ*, by the European programs.

Gas production in a clay repository is a potentially important process for creating permeability. However, gas production rates are very low relative to the gas injection rates used to produce macro-scale fractures in the oil and gas industry (NAGRA 2002). Like the behavior of salt, discrete pathways that may arise from gas overpressure form from slow "creep" deformation rather than brittle fracture processes. Once a pathway forms, the pressure is relieved by gas flow, and resealing occurs, until the pressure rises again (depending on gas supply). There is evidence that pathways in Opalinus clay reseal after gas breakthrough (NAGRA 2002), and this is also observed for Boom clay (Volckaert et al. 1995) and bentonite (Knowles and Howard 1996).

After resaturation of the repository, the hydrogeological situation will approach a pseudo-steady state, with the EDZ being self-sealed, the seals functioning as designed, and radionuclide migration effectively limited to diffusive transport through the (mostly undisturbed) clay/shale.

2.3.2 Coupled Thermal-Hydrologic-Mechanical (THM) Effects

Heating of the host rock will begin as soon as heat-generating waste is emplaced. Thermal response will be dominated by thermal expansion, principally of the pore water (which has 10 to 100 times more thermal expansivity than the solid framework). As discussed above, elevated pore pressure, combined with stress redistribution near excavated openings, reduces strength and increases deformation in clay/shale media. The potential contribution from thermal effects to the nature and extent of the EDZ is likely to be negligible if maximum temperature is limited (e.g., less than 100°C). Nevertheless, thermal response is being actively investigated at the European underground laboratories.

This section describes the responses of indurated clay/shale rock to heating, based on the published results from two *in situ* thermal tests. The discussion also reviews how thermal effects have been addressed in the preliminary performance assessments for repositories situated in these formations. This section includes a thermal analysis that evaluates the peak temperatures that would be produced in a typical soft shale formation from emplacement of HLW/UNF that has been identified for disposal in the U.S.

HE-D Experiment in the Opalinus Clay at Mont Terri, Switzerland – The HE-D experiment was begun in 2004 in the underground laboratory at Mont Terri to investigate the THM behavior of Opalinus clay in response to heating (Wileveau and Su 2007). A 30-cm diameter horizontal borehole was drilled to a total length of 14 m from a niche excavated off the main laboratory tunnel. Two electrical heaters, each 2 m long, were installed near the end of the borehole. A total of 24 measurement boreholes were drilled prior to the heater borehole, to observe the response to drilling and several months later, heating. An initial phase of heating, at approximately 160 W/m,

lasted for three months. Power was then increased to approximately 490 W/m for eight months. Measurements were conducted throughout the heating and subsequent cooling phases, and included temperature, deformation, deformation moduli, pore pressure, and gas permeability. After cooling, the test was dismantled for examination of the equipment and sampling of the rock.

Modeling and observations from the HE-D test (Jobman and Polster 2007; Gens et al. 2007) show that pore pressure responded immediately at the onset of heating, and was strongly correlated to local temperature. At a distance of approximately 1 m from the heater, the pore pressure increased from about 1 MPa to 4 MPa, corresponding to a temperature effect of 0.16 MPa/°C (Wileveau and Su 2007). After a few months, pore pressure measurements showed dissipation, probably by liquid flow. Pore pressure transients were correlated with reductions in unloading modulus measured using borehole dilatometry. Post-test sampling and mechanical testing revealed damage close to the heaters, but no significant damage over much of the region affected by thermally coupled pore pressure transients. These responses are consistent with recognition of an excavation-*disturbed* zone that has greater extent than the excavation-*damaged* zone (EDZ) in clay rocks, but which self-seals after the volume strain caused by the thermal transient subsides. Further extent of damage during cooling of the HE-D test was not observed.

TER Experiment in Callovo-Oxfordian Argillite near Bure, France – The TER experiment, begun in 2005, was similar to the HE-D test in the Opalinus clay, with instrumentation and heating of a pillar accessed by boreholes drilled from two perpendicular galleries. Similar instruments were installed, and as in the previous test, the heater borehole was drilled last to observe the rock mass response. Results from an initial 42-day heating period and subsequent seven months of cooling have been analyzed and reported in the literature (Wileveau and Su 2007). Observed deformations and pore pressure evolution were similar to the HE-D test. Thermally induced pore pressure increase was approximately 1.5 times greater than the preheating pore pressure. As in the HE-D test, at a particular location compression was observed first, followed by extension as the temperature field expanded.

Modeling of the TER test using an elasto-plastic Biot formulation (Jia et al. 2009) produced insights similar to those from the HE-D test. Modeling of viscous response (i.e., creep) was not needed because the test duration was only a few months. Analysis of results from the TER test (Jia et al. 2009) has confirmed that: (1) coupling of mechanical changes to thermal properties is insignificant; and (2) indurated clay formations such as the Callovo-Oxfordian argillite are stiff enough, and have low enough water content, that HM coupling effects on deformation are smaller than THM effects driven by thermal expansion.

Pore pressure in the TER test was observed to decrease steeply at the start of cooling, attributed mainly to thermal contraction of the pore fluid, and was simulated successfully. However, residual dilatancy from the effects of heating was proposed as an additional explanation for the steep changes (Jobmann and Polster 2007). Modeling of deformations observed in both the HE-D and TER tests (as reported to date) shows that deformation behavior is more complex than pore pressure. The effects of desaturation and inelastic consolidation on deformation are not well represented by existing models, although this does not preclude the eventual resaturation and sealing of clay host rocks over repository timeframes.

In summary, these two tests and the associated analyses show that the initial response to heating for a repository in clay/shale media would be dominated by thermal expansion, with dilatory thermal strain close to the waste packages, and compressional strain further away caused by outward thermal expansion. With time, the temperature field will expand so that the compressional strain becomes dilational. The region of elevated pore pressure may extend beyond the region of substantially elevated temperature because of the resulting stress distribution. Slight flow of liquid porewater in clay/shale media is apparently sufficient to dissipate excavation or thermally induced pore pressure transients.

As discussed above for hydro-mechanical coupling, increased pore pressure and drainage, combined with stress redistribution near excavated openings, will reduce strength and increase deformation. When cooling occurs, contraction of the pore fluid will cause desaturation, leading to increased suction (i.e., matric potential; Zhang and Rothfuchs 2007) leading to shrinkage of the solid framework. The associated gradient of matric potential will drive the eventual resaturation of the near-field environment. When the near-field host rock rehydrates (hundreds to thousands of years after cooling) the increased pore pressure will cause swelling, which will contribute to sealing. Permanent effects on rock characteristics will be limited in extent.

Coupled Thermal Effects in PA – Evaluations of the EDZ in the Opalinus clay (NAGRA 2002), and of the "micro-fissured zone" around openings in the Callovo-Oxfordian argillite (ANDRA 2005), indicate that the EDZ extent and its long-term properties will not be changed significantly by heating. For this assessment, the radial extent of the EDZ around access tunnels is limited to approximately 2 meters or less, and the long-term effective hydraulic conductivity of the EDZ is estimated to be approximately one order of magnitude greater than that of the undisturbed rock (Blümling et al. 2007; NAGRA 2002). Uncertainty with respect to the radial extent of the EDZ is mitigated in the performance analysis, by considering radionuclide mobility from the distal limit of the EDZ, outward into the undisturbed formation.

Clay-based swelling buffer materials (e.g., bentonite) are included in the NAGRA and ANDRA assessments. Although not considered here, such materials are available for backfilling around waste packages, and can achieve low permeability similar to undisturbed clay/shale rock while generating swelling pressure that acts to close voids in the near-field host rock.

Thermal Analysis of U.S. Waste Forms in Clay Media – The generic concept for HLW/UNF disposal used in this report relies on thermal conduction in the host rock to maintain maximum rock temperatures below boiling (e.g., less than 100°C). This will help avoid damage caused by dewatering and the associated shrinkage, and avoid pore pressure transients caused by boiling. This section presents a scoping thermal analysis that evaluates the peak temperatures at the emplacement borehole wall and the mid-point between emplacement boreholes, for ranges of emplacement borehole spacing and rock thermal conductivity (K_{th}). This analysis uses an analytical solution for line-source heating, with superposition to represent time-dependent repository heating (SNL 2008a, Section 6.1), following an approach used extensively in the thermal management strategy for the Yucca Mountain repository license application (DOE 2008, Section 1.3.1.2.5). It considers a range of waste thermal output, from older HLWG (Hanford), to a limiting case that bounds the heat output from relatively young ("hottest average") used PWR fuel from commercial reactors. The results show the range of temperatures achievable with the generic clay/shale repository.

The most important rock parameter for predicting repository temperatures is thermal conductivity; heat capacity is relatively unimportant because of the long time scale. Analysis of test results from clay/shale media indicates significant anisotropy, with K_{th} more than 50% greater in the direction parallel to bedding compared to the direction perpendicular to bedding (Table 2.3-1). For this scoping analysis, an isotropic K_{th} value of 1.45 W/m-K is derived from the geometric mean of the horizontal (parallel) and vertical (perpendicular) reference values for the Opalinus clay (Gens et al. 2007). The range of heat capacity indicated in Table 2.3-1 has a negligible influence on peak temperatures in this analysis.

Formation	Thermal Conductivity (W/m-K)	Heat capacity (J/kg-K)	Method	Source
Opalinus	1.70 0.81 ⊥	920	Back-calculation	Jobmann and Polster 2007
	2.8 1.6⊥	840	Back-calculation	Gens et al. 2007
	3.2 ∥ 1.8 ⊥ 1.5 EDZ		Estimated	Johnson et al. 2002
	2.1 ∥ 0.995⊥	800	Reference	Gens et al. 2007
Callovo- Oxfordian	1.75	1005	(typical)	Jia et al. 2009

Table 2.3-1. Thermal Properties for Opalinus and Callovo-Oxfordian Formations

Heat output for UNF and HLWG is taken from a thermal loading analysis prepared for the Yucca Mountain repository license application (SNL 2008a). Thermal decay curves for waste packages containing either 21 PWR UNF assemblies, or five HLWG (Hanford) canisters, were divided by the respective numbers of canisters to obtain curves for single-assembly or single-canister waste packages such as would be emplaced in a clay/shale repository. The 21-PWR decay curve was selected to represent typical UNF with age 5 years out-of-reactor, while the HLWG decay curve is typical for Hanford glass (which has already undergone approximately 40 years of decay storage). Thus, these are end members representing the hottest and coolest waste forms that currently exist and would be emplaced in a clay/shale repository. In the analysis, these waste forms are emplaced within 1 year of transport to the repository (no decay storage prior to emplacement, or ventilated period after emplacement). Peak temperatures are calculated for the mid-point between any two horizontal emplacement boreholes, and for the emplacement borehole wall.

The solution is recalculated for ranges of emplacement borehole spacing and host-rock K_{th} (Figures 2.3-1 and 2.3-2). The results show that the heat output from Hanford HLWG (representing waste from once-through reprocessing that recovers Pu, with approximately 50 years of decay storage) is negligible for disposal in clay/shale media. For older HLWG, the emplacement borehole spacing could be as small as a few meters. Younger HLWG with greater heat output would not change this result significantly. For UNF, the reference borehole spacing of 20 m is sufficient to limit both the midpoint and borehole wall temperatures (e.g., less than 100°C) for effective thermal conductivity as small as 1.4 W/m-K, thus covering much of the

range of K_{th} shown in Table 2.3-1. Additional flexibility is provided by the possibility of HLWG or UNF decay storage prior to emplacement. This analysis demonstrates that the reference clay/shale concept is feasible with respect to meeting *in situ* temperature limits for disposal of the present U.S. HLW/UNF inventory, and with decay storage has the flexibility to meet those limits for other possible waste forms.

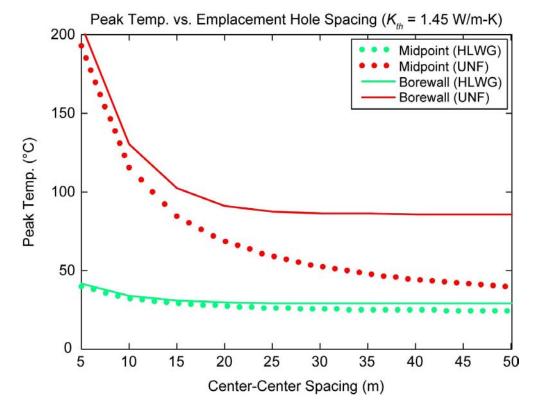


Figure 2.3-1. Peak Postclosure Temperatures for the Generic Disposal Concept in Clay/Shale, as a Function of Emplacement Borehole Spacing, for Young PWR UNF and Cooler HLWG

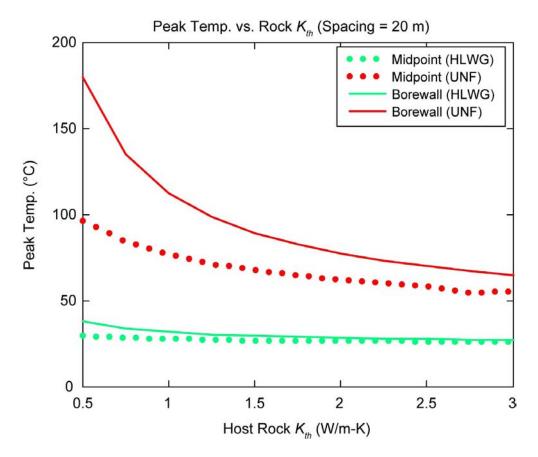


Figure 2.3-2. Peak Postclosure Temperatures for the Generic Disposal Concept in Clay/Shale, as a Function of Host Rock Thermal Conductivity (K_{th}), for Young PWR UNF and Cooler HLWG

2.3.3 Far-Field Responses of the Host Rock and Overlying Strata

With effective drift closures and shaft seal systems, radionuclide transport in the far-field host rock would be limited by low permeability, so that diffusion is the dominant transport mechanism for 1,000,000 years or longer. Both liquid and gaseous advection are limited by intrinsic permeability on the order of 10^{-19} m² or less (Section 2.2.1). The presence of overpressured fluid in the Opalinus clay (estimated to have head as much as 100 m greater than a water column to the ground surface; NAGRA 2002) gives strong evidence of low permeability. For this excess head to persist over geologic time signifies that advective transport is not significant in the repository time frame.

The existence of overpressure has been used as the basis for alternative PA scenarios in which transport (either in the EDZ or the host rock) is driven by hydraulic gradients over short distances (Section 3.2, Scenario 1; also see NAGRA 2002). These cases may be unrealistic because they are based on head differences only, without considering the difficulty of producing sufficient fluid to overcome fluid uptake within the repository (e.g., hydration), or to drive significant advective transport of radionuclides out of the repository. There is the potential for faults, fracture zones, or other structural features to exist in shales. Such features have been studied at both the Meuse/Haute-Marne (Callovo-Oxfordian) and Mont Terri (Opalinus) sites,

and are evaluated in the respective preliminary performance assessments (ANDRA 2005; NAGRA 2002).

Indurated clay formations exist in the U.S. that are at least as thick as those being considered in Europe (Boisson 2005, Figures 1 and 2). Within the nominal scenario class, the largest driving force for fluid flow and radionuclide migration away from a clay/shale repository may be thermally induced pore pressure transients. However, the duration of the thermal pulse will likely be much less than the effectiveness of the engineered barriers, or of the natural barrier beyond the influence of repository-induced temperature changes. Although heating tends to drive water away from the repository to mobilize radionuclides, but can do so only after cooling, and after rehydration.

2.4 Coupled Multi-Physics Analyses for a Generic Clay/Shale Repository

This section presents the results of coupled thermal-hydrologic-mechanical-chemical (THMC; THM with chemical transport) calculations for a generic repository in clay/shale. The problem was chosen to demonstrate the current capabilities of the SIERRA Mechanics software (Edwards 2002) as applied to a repository problem that requires many of the software's unique capabilities. The geometries, material properties, thermal loading, and other features of these calculations were chosen to be represent potential repository designs.

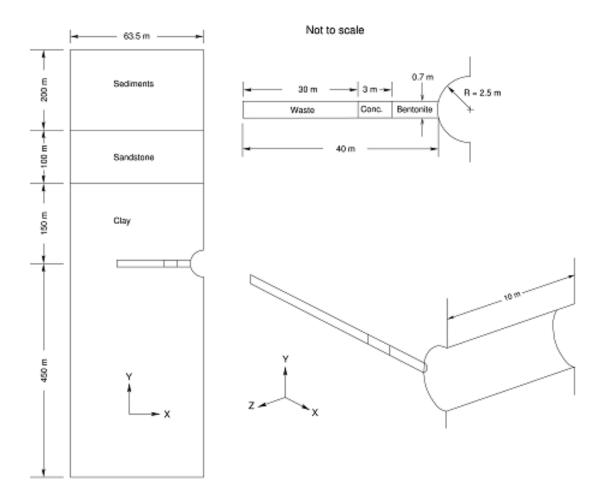
The development of the SIERRA Mechanics code suite has been funded by the Department of Energy (DOE) Advanced Simulation and Computing (ASC) program for more than ten years. The goal is development of massively parallel multi-physics capabilities to support the Sandia engineering sciences mission. SIERRA Mechanics was designed and developed to run on the latest and most sophisticated massively parallel computing hardware, with capability to span the hardware range from single workstations to systems with thousands of processors. The foundation of SIERRA Mechanics is the SIERRA toolkit, which provides finite element application-code services such as: (1) mesh and field data management, both parallel and distributed; (2) transfer operators for mapping field variables from one mechanics application to another; (3) a solution controller for code coupling; and (4) included third party libraries (e.g., solver libraries, communications package, etc.).

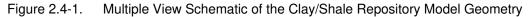
The SIERRA Mechanics code suite comprises application codes that address specific physics regimes. The two SIERRA Mechanics codes that are used for THMC coupling are Aria (Notz et al. 2007) and Adagio (Jung et al. 2009). The physics currently supported by Aria include the incompressible Navier-Stokes equations, energy transport equation, and species transport equations, as well as generalized scalar, vector, and tensor transport equations. The multi-phase porous flow capability is a recent addition to Aria. Aria also has some basic geochemistry functionality available through embedded chemistry packages. The mechanics portion of the THMC coupling is handled by Adagio, which solves for the quasistatic, large deformation, large strain behavior of nonlinear solids in three dimensions. Adagio has some discriminating technology, developed at Sandia for solving solid mechanics problems, that involves matrix-free iterative solution algorithms for efficient solution of extremely large and highly nonlinear problems. This technology is especially suited for scalable implementation on massively parallel computers. The THMC coupling is done through a solution controller within SIERRA

Mechanics called Arpeggio. Sandia's Laboratory Directed Research and Development program has been the major funding source for the SIERRA Mechanics THMC development.

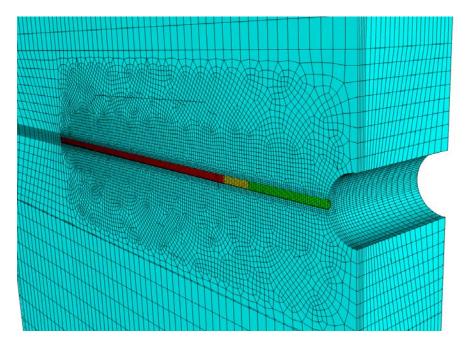
In this section, we present the results from THMC simulations of a generic waste repository sited below the water table in a clay layer. The repository configuration and heat generation are described in Sections 2.1 and 2.3, respectively, and are chosen to represent potential designs but are not meant to specify an actual design. The material properties used in this work represent relevant geologic materials, but are not site specific nor based on measured data from any one site.

The model geometry defines a "unit cell" model of a hypothetical waste repository sited in a 600-m thick clay/shale layer overlain by 100 m of sandstone and 200 m of other sediments (Figure 2.4-1). The entire domain is 900 m deep, 63.5 m wide, and 10 m in the horizontal direction perpendicular to the page. The repository is situated 150 m within the clay layer. Repository workings are represented by a horizontal, 5-m diameter access tunnel, with a perpendicular, 0.7-m diameter, 40-m long horizontal emplacement borehole. The waste packages occupy the distal 30 m, followed by a 3-m concrete plug, and finally a 7-m bentonite seal flush with the wall of the access tunnel.





The Adagio mechanical analysis and Aria thermo-hydrological-chemical analysis used the same finite element mesh discretization. It should be noted that this is not required, as Arpeggio is capable of interpolating information between different meshes and geometries. A detail of the mesh at the repository horizon is shown in Figure 2.4-2. The finite element grid consists of 404,076 nodes and 383,214 eight-node hex elements. The analysis was run on a multi-processor computer using 32 processors requiring approximately five hours of computer time for 10,000 years of simulation time.



NOTE: The stored waste (red), concrete plug (yellow), and bentonite (green) materials are shown in the borehole. Figure 2.4-2. Finite Element Mesh Detail at the Waste Horizon Showing the Access Tunnel and Horizontal Waste Borehole

2.4.1 Mechanical Model Definition

The geometry shown in Figures 2.4-1 and 2.4-2 represents a "3D slice" from the repository. The vertical planes in the model are symmetry boundaries with normal displacements fixed against horizontal movement. The base of the model is fixed against vertical movement. The geologic materials – clay, sandstone, and sediments – are set to an initial hydrostatic stress condition (the horizontal normal stresses are equal to the vertical overburden stress). The applied external forces are body forces associated with weight of the overburden. Excavation of the access drift and emplacement boreholes is simulated by releasing the initial normal stresses at the free surfaces, over a construction period of one day. After excavation, the thermal loads and water vapor pressures are transferred from Aria and the coupled calculation is run out to 10,000 years. Deformations resulting from the mechanical analysis are transferred to the THC model).

Material property inputs are listed in Tables 2.4-1 and 2.4-2. With the exception of the clay layer, the stratigraphic materials were modeled as linear elastic. The clay materials, the entire clay layer, and the bentonite plug are modeled using the crushable soil and foam material model in

Adagio. At present, Adagio does not have a clay specific material model implemented. The mechanical properties for the waste canisters, except for the density, are based on the properties of steel. The intent is to have the waste canisters behave as nearly rigid bodies within the clay.

Property	Waste Canister	Concrete Plug	Typical Sandstone	Surficial Sediments	Units
Density	1256.7	2247.3	2100	1800	kg/m ³
Young's Modulus	4.32	23.87	23.0	0.145	GPa
Poisson Ratio	0.3	0.2	0.3	0.2	—
Coefficient of Thermal Expansion	11.7E-06	12.0E-06	11.6E-06	11.6E-08	C° ^{−1}

Table 2.4-1. Physical and Elastic Material Properties

Sources: Holland 2008; ACI 1978; Bowles 1976.

NOTE: Concrete Young's modulus is estimated from ACI (1978) formula: $E = w^{1.5} 33 \sqrt{f'_c} \quad lb_f / in^2$ with weight density ($w = 140 \quad lb_f / ft^3$) and unconfined compressive strength $f'_c = 4,000 \quad lb_f / in^2$

Property	Bentonite (Backfill/buffer)	Clay Formation	Units
Density	1700	2700	kg/m ³
Young's Modulus	7.00E+07	7.50E+09	Pa
Poisson Ratio	0.2	0.295	(dimensionless)
<i>a</i> ₀	3.45E+06	3.45E+06	Pa
a ₁	0	0	(dimensionless)
a ₂	0	0	Pa ⁻¹
Cut-off Pressure -2.07E+06		-2.07E+06	Pa
Coefficient of Linear Thermal Expansion See note		14.0E-06	m/m-C°

Table 2.4-2.	Bentonite and Clay	Properties for the	Crushable Soil and	Foam Model
	Demonite and Oldy		orabilable oon and	

Sources: Sobolik et al. 2002; Gens et al. 2007.

NOTE: Temperature strain function for bentonite (T in Kelvin):

$$\varepsilon_T = 3.25E - 06T^2 - 1.18E - 05T - 3.26E - 04 \quad (m / m - K^{\circ})$$

For the soils and crushable foam model in Adagio, the assumed yield surface is a surface of revolution about the hydrostat in principal stress space. In addition, a planar end cap on the normally open end of the surface of revolution is assumed. The yield stress is specified as a polynomial in pressure, p (positive in compression):

$$\sigma_{yd} = a_0 + a_1 p + a_2 p^2$$
 (Eq. 2.4-1)

For this particular analysis, a_0 is non-zero, and a_1 and a_2 are specified to be zero, which results in an elastic-perfectly plastic deviatoric response. This makes the yield surface a cylinder oriented along the hydrostat in principal stress space. The plasticity theories for the volumetric and deviatoric parts of the material response are completely uncoupled. The mean pressure, p, is assumed to be positive in compression, and a yield function is written for the volumetric response as $\phi_p = p - f_p(\varepsilon_v)$ where $f_p(\varepsilon_v)$ defines the volumetric stress-strain curve for the pressure. The deviatoric part of the response is computed using a conventional plasticity theory with radial return to compute the stress at the end of the step.

2.4.2 Thermal-Hydrologic Model Definition

The thermal-hydrologic boundary and initial conditions are summarized in Figure 2.4-3. Initially, the entire domain is assumed to be at 20°C and initial saturation corresponding roughly to a (hydrologic) steady state with the upper surface set to 25% liquid saturation. This steady solution was computed separately, and results in nearly uniform saturations in each material, away from material interfaces. These steady saturations were applied as initial saturations in each material for the heat-driven simulation, with values as depicted in Figure 2.4-3.

The top of the domain represents the ground surface and was set to a temperature of 20°C and a liquid saturation of 25%. The bottom boundary temperature was also set to 20°C. The access tunnel was assumed impermeable to flow and was subject to a natural convection boundary condition, representing a non-backfilled configuration for the duration of the thermal pulse, with 20°C reference temperature (Figure 2.4-3). All other surfaces were specified as symmetry surfaces, impermeable to mass flow and insulated from heat flow. For the HLWG case, the initial saturation of the host rock was 61%, and this saturation condition was also maintained at the bottom boundary. For the PWR UNF cases (discussed below), the initial saturation was increased to 91% to evaluate the potential for pore pressure excursions and the associated mechanical responses.

The thermal-hydrologic model assumes that unsaturated porosity is occupied by liquid water and water vapor. Air is not considered in the present model. The mass balance for water includes pressure-driven flow (including thermally driven flow), gravity, evaporation/condensation, and capillary pressure between liquid and its vapor. The energy transport equation includes two phase (liquid and gas) mass flow driven convection of sensible and latent heat (evaporation and condensation), heat conduction and buoyancy, and heat generation from the waste package.

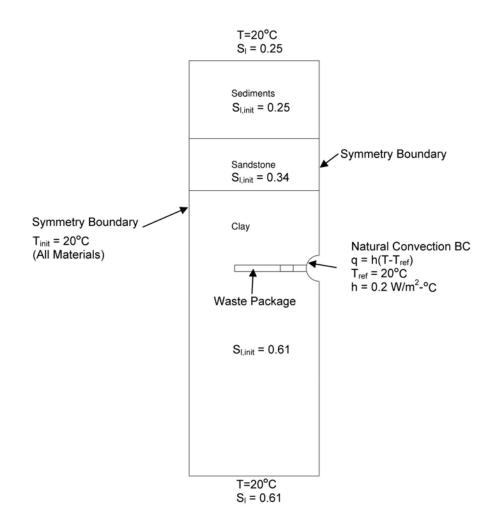
The waste package region is a cylindrical domain, assumed to be composed of the clay material, but with uniform volume generation of decay heat. The domain is 0.7 m in diameter and 30 m long (11.5 m^3) .

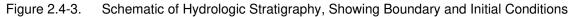
Three different thermal loads are used in the analyses, to represent: (1) fresh HLWG; (2) the hottest PWR UNF considered for the Yucca Mountain license application; and (3) a bounding case for PWR UNF:

• The HLWG thermal power decays with a half-life of about 30 years (representing ¹³⁷Cs and ⁹⁰Sr) and rapidly decays to insignificance. For this case the power density for Hanford HLWG was scaled up to represent fresh HLW, such that peak emplacement

temperatures approach but do not exceed boiling. This condition was chosen to maximize evaporation and condensation behavior in the near field, without exceeding 100°C.

- The hottest PWR UNF case is based on the average base case thermal PWR UNF thermal output used in performance assessment analyses to support the Yucca Mountain license application, which was then scaled up to envelop the estimated limiting waste stream (ELWS) PWR UNF used for the Yucca Mountain analysis (DOE 2008, Section 1.3.1.2.5). It thus represents commercial UNF with the greatest thermal decay energy density that was considered for the license application (SNL 2008a, Section 6.1).
- The bounding case was developed by scaling up the Yucca Mountain ELWS by approximately 180%, to represent possible hotter, future waste forms. When decay storage is implemented for 50 years prior to emplacement, this bounding case resembles the HLWG case (Figure 2.4-4).





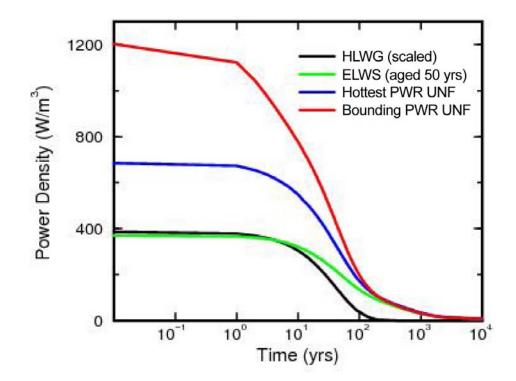


Figure 2.4-4. Normalized Power Curve for HLWG Waste Used in the Clay/Shale Repository Calculations

Thermal-Hydrologic Material Properties and Flow Models – Material properties and parameters applied in the model are given in Table 2.4-3. Again, these values are within a realistic range of values for the type of porous material. Note that the porosity of the clay/shale formation is assigned a large value (30%) to investigate the potential for pore water and vapor mobilization. The permeability of the clay/shale formation is assigned a value of 10^{-16} m² for the HLWG case, and 10^{-19} m² for the hottest PWR UNF and bounding cases, reflecting a progression of cases intended to explore the maximum range of pore pressure and mechanical responses.

Property	Clay Formation	Typical Sandstone	Surficial Sediments	Concrete Plug	Bentonite (Backfill/buffer)	Units
Porosity	0.3	0.2	0.4	0.1	0.276	(dimensionless)
Permeability	10 ⁻¹⁶ to 10 ⁻¹⁹	10 ⁻¹⁵	7×10 ⁻¹⁴	10 ⁻¹⁸	2.6×10 ⁻¹⁹	m²
Thermal Diffusivity	1.04×10^{-6}	$1.40 imes 10^{-6}$	1.05×10^{-6}	$4.55 imes 10^{-7}$	1.00×10^{-6}	m²/sec
VG P _{c0}	10	10	8.63	10	10	kPa
VG β	1.69	1.69	1.88	1.69	1.69	(dimensionless)
Sr	0.11	0.11	0.2	0.11 ^a	0.11	(dimensionless)

Table 2.4-3. Thermal-Hydrologic Material Properties

^a Residual liquid saturation = 0.005 in relative permeability model.

Curve fits to thermodynamic properties for water (liquid and vapor) are used in the model. The parameters VG P_{c0} and VG β refer to the van Genuchten (1980) model. Capillary pressure, P_c , as a function of liquid saturation, *s*, was specified as:

$$P_{c} = P_{c0} \left(s^{-1/\lambda} - 1 \right)^{1/\beta}, \quad \lambda = 1 - 1/\beta$$
 (Eq. 2.4-2)

where the scaled liquid saturation is defined by,

$$s = (S_l - S_r)/(1 - S_r)$$
 (Eq. 2.4-3)

and S_l denotes the liquid saturation and S_r the residual liquid saturation.

The Udell cubic function of liquid saturation was used to specify relative permeability for all materials:

$$k_{rl} = s^3$$

 $k_{rg} = (1-s)^3$ (Eq. 2.4-4)

2.4.3 Chemical Model Definition

Boundary conditions for the geochemical model are similar to those used for the thermalhydrologic model (see Figure 2.4-3). Boundary values of concentration at the top and bottom of the domain are set to zero. Boundary conditions at the sides of the domain are symmetry conditions as described in the previous section. Initially, the entire domain is chosen to have zero concentration, except for the waste package region, which is taken to be equal to unity. The tracer in these calculations decays with a half-life of 30.1 years (¹³⁷Cs), which is consistent with the thermal loading rate discussed in the previous section. Details and parameter values assumed in the geochemical modeling portion of the study are discussed in a later section.

2.4.4 Thermal-Hydrologic-Mechanical Model Results

Mechanical calculations are important for assessing the structural integrity of the access tunnel and waste borehole. The tunnel excavation occurs over several solution steps prior to the start of waste heating. Figure 2.4-5 shows color contour plots of maximum principal stress at the end of the excavation period. The plots show an area of tensile stress that exists in the access tunnel roof and floor at the location of the emplacement borehole. This location is unique due to the intersection of two symmetry planes (x- and z-directions). The constraint of the kinematic boundary conditions on two sides plus the inelastic material response of the clay produces the tensile stress field. This was verified by simulating the excavation sequence using a linear elastic material for the clay. No tensile stresses were observed in the tunnel roof and floor for the linear elastic clay model. This illustrates the need for appropriate, site-specific material models for the clay/shale to get accurate stress results for tunnel integrity assessment. This result shows the value of three-dimensional calculations and clearly identifies an area for further evaluation.

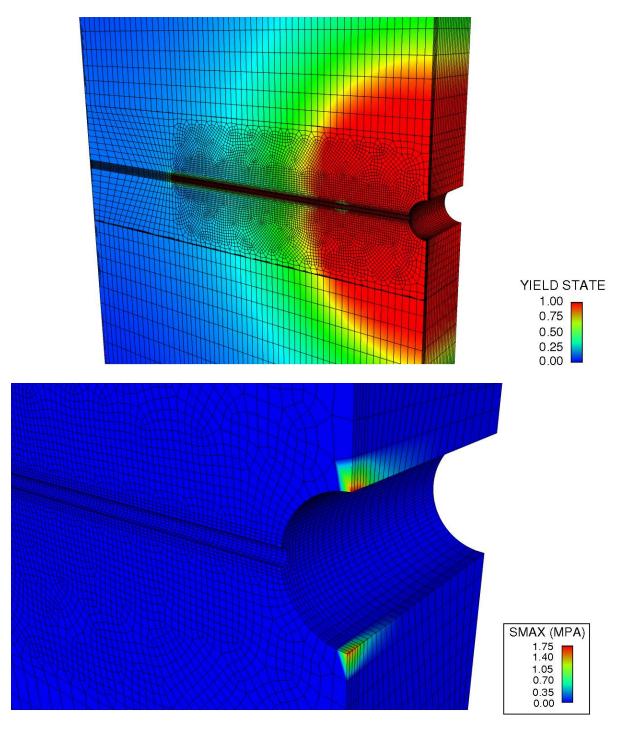


Figure 2.4-5. Color Contour Plots of Post-Processed Yield State Variable and Maximum Principal Stress (SMAX) after Access Tunnel Excavation

Figure 2.4-5 also shows the volume of clay material that is exhibiting nonlinear material response. The plotted yield state quantity (upper plot) is the non-dimensional ratio of the computed von Mises stress divided by the a_0 constant in the constitutive model. If the ratio is less than 1.0, then the material is elastic, and if equal to 1.0, the material is inelastic (stress state is on the yield surface). This figure indicates that the zone of inelastic response extends to a distance of several diameters surrounding the access tunnel, but not the emplacement borehole. The shape and extent of this region, and the relationship between the extent of transient rock disturbance and the permanent EDZ, depend on the constitutive models used for the clay, and would be subject to further, site-specific investigations.

The peak emplacement borehole temperatures range from 83.5°C for the HLWG case, to greater than 200°C for the bounding case (Figures 2.4-6 and -7). Although the peak temperatures for the PWR cases exceed 100°C, these responses can be readily changed using decay storage as discussed in Section 2.3.2. For the HLWG case with relatively small temperature changes, thermal expansion of the solid matrix has a very small effect on the stress state. Also, displacements near the access tunnel are small. From these calculations, the largest structural response of the clay surrounding the access tunnel and emplacement borehole apparently occurs during excavation.

All of the thermal power decay histories are defined such that the repository dries out noticeably within a few years, then re-wets as the repository cools down. For the HLWG case with greater rock permeability $(10^{-16} \text{ m}^2; \text{Table 2.4-3})$, water is evaporated near the emplacement borehole, driven away by vapor pressure gradients, and condenses further out, forming a zone of increased saturation. Capillary gradients support liquid flow back toward the borehole. Where this flow impinges on the borehole from above, a zone of increased saturation forms above the borehole but not below (Figure 2.4-8). Note that the initial saturation of the host rock was set to 61% for this simulation.

For the PWR UNF cases with lower permeability (10^{-19} m^2) , the dewatering response occurs but the subsequent flow is virtually absent, as indicated by the vertical symmetry of saturation profiles (Figure 2.4-8). Pore pressure response closely follows the vapor pressure of water (Figure 2.4-7), with some dissipation especially for the HLWG case with greater permeability. Note that the initial saturation of the host rock was set to 91% for these simulations.

The spatial extent of elevated pore pressure and the time scale for dissipation are demonstrated for the bounding PWR UNF case in Figure 2.4-9. Noting that this is a bounding case for which peak temperature greatly exceeds 100°C (Section 2.3.2), this result shows that the duration of elevated temperatures is limited and the thermal gradients in the rock are small beyond a few meters distance. Thermodiffusion (Soret effect) can therefore be excluded as a significant radionuclide transport process (SNL 2008b, FEP 2.1.11.10.0A).

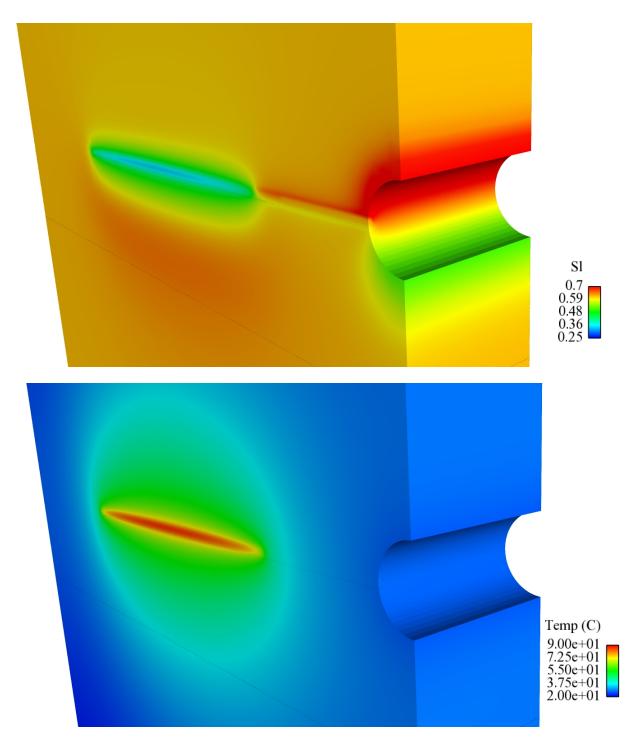


Figure 2.4-6. Liquid Saturation (S_i) and Temperature Distributions near the Waste Packages at 16 Years, for the Fresh HLWG Thermal Case

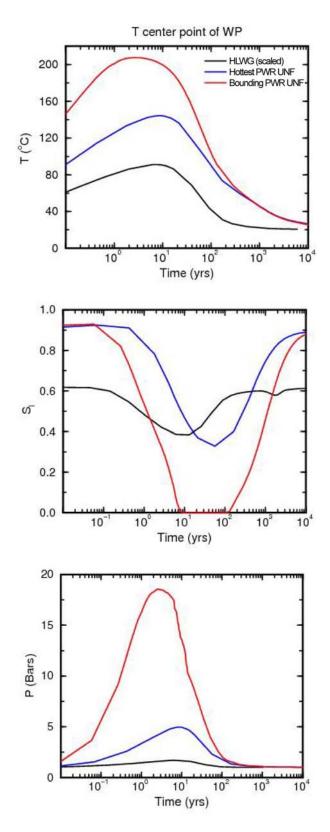
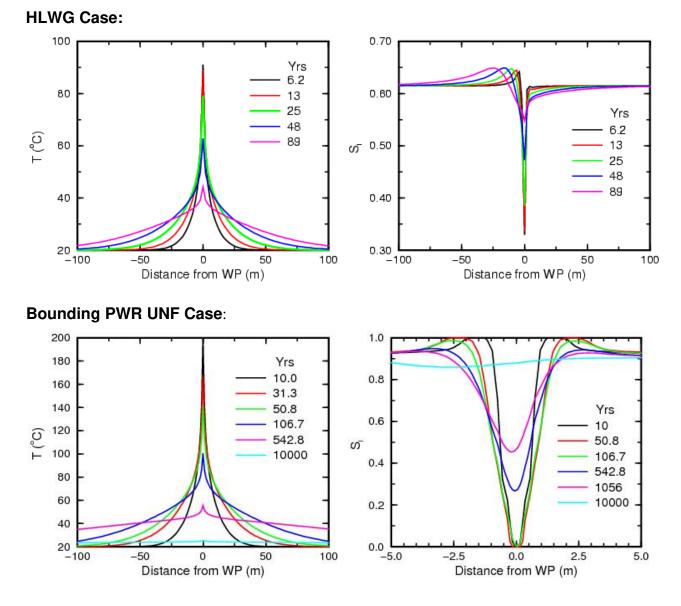


Figure 2.4-7. History of Temperature in the Emplacement Borehole (upper); History of Liquid Saturation in the Emplacement Borehole (middle); and History of Pore Pressure in the Emplacement Borehole (lower)



- NOTE: The vertical transect cuts through middle of the 30-m long region where waste packages are emplaced. Negative distance extends above the emplacement borehole, and positive distance below it.
- Figure 2.4-8. Temperature (T) and Liquid Saturation (S_I) Distribution as a Function of Vertical Distance from the Waste Package, for the Fresh HLWG Thermal Case (upper) and the Bounding PWR UNF Case (lower)

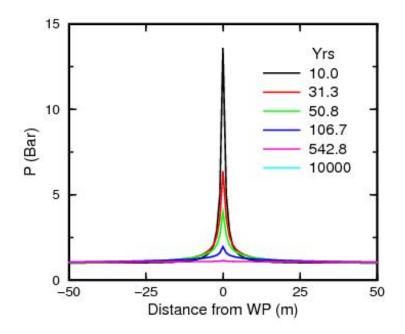


Figure 2.4-9. Pore Pressure Response as a Function of Vertical Distance from the Waste Package, for the Bounding PWR UNF Case

2.4.5 Geochemical Modeling and Results

Transport of a single radionuclide is modeled using a simple formulation with first-order radioactive decay and adsorptive retardation, which is part of the present SIERRA Mechanics suite.

Conservation of mass for the *i*th aqueous or gaseous solute mass (c_i is the molar concentration) in a phase π with saturation *s* and porosity ϕ is given by

$$\frac{\partial}{\partial t} \left(\phi s_{\pi_i} c_i \right) + \vec{\nabla} \cdot \vec{J}_i = \sum_{r=1}^{N_r} v_{ir} I_r \quad (i = 1, \dots N)$$
(Eq. 2.4-5)

with flux J. The sum on the right hand side is over the total possible N_r homogeneous and heterogeneous reactions I_r in π , where v_{ir} are the stoichiometric coefficients (number of moles of *i* participating in the *r*th reaction). We consider only a single aqueous solute species with concentration *c*, and account for advective and diffusive flux, so that Equation 2.4-5 becomes

$$\frac{\partial}{\partial t}(\phi s_L c) + \vec{\nabla} \cdot (\vec{v}_L c) = -\vec{\nabla} \cdot (\phi s_L D \vec{\nabla} c) + \phi R \qquad (\text{Eq. 2.4-6})$$

Here v_L is the liquid Darcy velocity and D is an effective mass diffusion coefficient that includes tortuosity but not porosity or liquid saturation (i.e., $D = D_m t$). Variable R is the net molar production rate of c, which for our purposes consists of a term accounting for first-order radioactive decay and a term accounting for sorption. Following the treatment by Schwartz and Zhang (2003, Equation 23.12), then Equation 2.4-6 becomes

$$\frac{\partial}{\partial t}(\phi s_L c) + \vec{\nabla} \cdot (\vec{v}_L c) + \frac{\partial}{\partial t}(sa_m) = -\vec{\nabla} \cdot (\phi s_L D \vec{\nabla} c) + r \qquad (\text{Eq. 2.4-7})$$

where the third term on the left-hand-side is the time rate of change of the product of an areal molar concentration *s* and the specific surface area of mineral per unit bulk volume, a_m , and *r* accounts for any other chemical reaction rate. When sorption reaction rates are considered rapid relative to transport rates, *s* will reflect a local equilibrium with the local bulk fluid concentration *c*, and thus can be represented by a sorption isotherm. Assuming a simple linear isotherm (linear relation between *c* and *s*) permits the introduction of a retardation factor R_f in Equation 2.4-7 such that

$$\frac{\partial}{\partial t}(\phi s_L c R_f) + \vec{\nabla} \cdot (\vec{v}_L c) = -\vec{\nabla} \cdot (\phi s_L D \vec{\nabla} c) + r$$
(Eq. 2.4-8)

where $R_f = 1 + a_m k/\phi s_L$ with k the isotherm constant. Usually retardation is defined in terms of an apparent distribution coefficient (as a means of relating sorption behavior to experimental measurement) k_d , which relates the total contaminant mass adsorbed per total solid mass to the bulk aqueous concentration. With $k_d = a_m k/\rho_b$ and ρ_b the bulk mass density, $R_f = 1 + \rho_b k_d/\phi s_L$ (Equation 23.14 of Schwartz and Zhang 2003, here modified for partially saturated media).

For a solute species undergoing first-order radioactive decay, $r = -\phi s_L R_f \lambda c$, where λ is the decay constant, related to radionuclide half-life by $t_{1/2} = ln(2)/\lambda$ (Schwartz and Zhang 2003, Equation 23.16).

Solution in Aria – To solve Equation 2.4-8 for relevant boundary and initial conditions, and to include this in a multi-physics treatment that couples solute transport with multi-phase flow and mechanics, we use Aria. Presently, the solute reaction and transport solver within Aria (the SPECIES capability based on conservation of chemical species mass) requires a constant porosity and saturation, and for our problem, a constant retardation factor. With these assumptions, assuming further a constant *D*, and with λ and R_f defined as discussed above, Equation 2.4-8 becomes

$$\frac{\partial c}{\partial t} - \frac{1}{R_f \theta} \vec{\nabla} \cdot (\vec{v}_L c) = \frac{D}{R_f \theta} \nabla^2 c - \lambda c$$
 (Eq. 2.4-9)

where the liquid moisture content $\theta = \phi s_L$. This is a form readily solved by Aria.

Parameters – Solving Equation 2.4-9 requires values for the four parameters R_f , θ , D, and λ , which in turn requires estimates for the distribution coefficient k_d , the free-liquid mass diffusion coefficient D_m , tortuosity τ , half-life $t_{1/2}$, bulk density ρ_b , porosity ϕ , and liquid saturation s_L . These would be considered average values over the spatial and temporal simulation domains. Considering the case of reaction and transport of ¹³⁷Cs in a clay-bearing country rock, reasonable values for these parameters are:

 $k_d = 320 \text{ mL/mg}$ (consistent with the range from Table 2.3-2) $D_m = 1.64 \times 10^{-9} \text{ m}^2/\text{sec}$ $t_{1/2} = 30$ years (representing ⁹⁰Sr or ¹³⁷Cs) $\rho_b = 2.22$ g/cm³ $\theta = .05$ and $\tau = 0.5$ (estimates)

These values yield $(R_f \theta)^{-1} = 0.0014$; $D/R_f \theta = 1.15 \times 10^{-12} \text{ m}^2/\text{sec}$; and $\lambda = 7.32 \times 10^{-10} \text{ sec}^{-1}$.

Results – Because of the short half-life and relatively large retardation factor used in this calculation, transport times are short relative to decay times. This is evident in Figure 2.4-10, which plots a normalized or scaled concentration as a function of time. Initially, the scaled concentration is unity inside the waste package region (Figure 2.4-3). Parameter values are such that, for ¹³⁷Cs, a concentration of unity would be about 10^4 mg/L. After 5 years the concentration profile shows a very small migration, on the order of centimeters. Twenty years out, the concentration profile begins to narrow at the center, associated with radioactive decay but also with the relatively larger liquid advective velocity (because of the larger spatial gradients in liquid saturation and heat in this region, during this time). By approximately 30 years, sufficient radioactive decay has led to the near disappearance of solute in this region, and by 60 years (not shown), the solute has nearly disappeared from the solution. This result shows that fission products comprising the constituents of HLW that have the greatest specific activities (and shortest half-lives) are completely isolated from the geosphere overlying the simulated clay/shale repository.

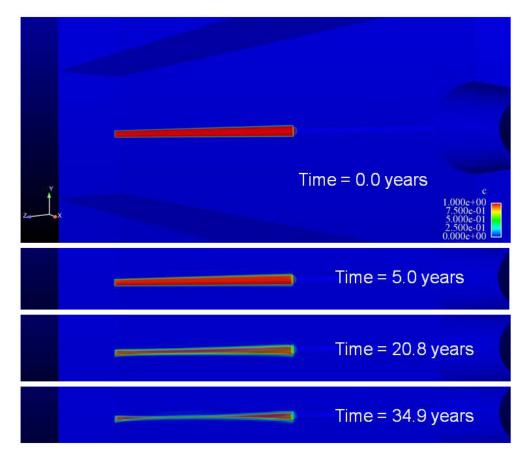


Figure 2.4-10. Normalized or Scaled Concentration of ¹³⁷Cs near the Waste as a Function of Time

2.4.6 Multiphysics Modeling Summary

Results presented in the foregoing sections are generally consistent with calculations performed by international programs, particularly ANDRA and NAGRA, and discussed in Section 2.3. The calculations confirm the result presented in Section 2.3, that the maximum host rock temperature can be limited (e.g., less than 100°C) by selection or decay storage of waste forms. The duration of elevated host rock temperatures would be limited to a few hundred years, during which substantial dewatering of the near-field host rock could occur, given sufficient permeability. The region of plastic deformation and stress conditions modified by excavation could be dominated by the larger diameter access drift. The extent of the EDZ would be sensitive to site-specific rock constitutive behavior, but the results from these generic simulations are consistent with a maximum extent of a few meters. The behavior of ¹³⁷Cs in radionuclide transport simulations represents the isolation, and attenuation by radioactive decay, that is expected for disposal in clay/shale formations. Based on these results, and EDZ investigations by international programs (Section 2.3.1), the extent of the EDZ is limited to a few meters and can be ignored as a transport path segment in the performance analysis of a generic clay/shale repository.

2.5 Chemical Environment

The geochemical behavior (solubility, sorption, colloidal behavior, etc.) of the projected waste inventory (Appendix A) in clay/shale media would limit the rate of degradation of the uranium oxide UNF matrix, and limit the potential for radionuclide transport to the biosphere. Degradation rates for UNF would be limited because of reducing conditions and very low advective liquid flux within clay/shale formations. Radionuclide releases from the waste form would be further limited by low solubility phases (e.g., simple reduced oxides of the actinides). Transport through the clay/shale formation would be strongly retarded for some radioelements via sorption and/or cation exchange with clay minerals. Radionuclide-bearing phase solubilities and sorption coefficients are important input parameters for the generic performance analysis (Section 4).

Fluids in contact with clay/shale media tend to be rich in sodium, calcium, and chloride. Lesser amounts of sulfate and carbonate are likely to be present. For the purpose of estimating radionuclide solubilities, we use a 0.7 mole/L NaCl solution with pH of 7 at a system E_H of approximately -300 mV and a temperature of 100°C. This solution composition provides an idealized starting point for estimates of solubility-limited radionuclide concentrations. Given the elevated temperature of the calculation, this idealized composition is somewhat more concentrated and has a slightly lower pH compared to some analyzed argillaceous porewater compositions for the Opalinus clay or extracted from bentonite of the FEBEX tests (see Table 1 of Metz et al. 2003). The low redox state reflects control of low oxidation potential by the presence of pyrite and organic carbon in the shales, as well as by reaction of the steel canisters containing the waste forms.

The pH of the waters in clay/shale systems would tend to be buffered by reactions with carbonate phases, to slightly alkaline values, and to a lesser extent by surface protonation/deprotonation reactions of clay minerals. These characteristics, with a high capacity for buffering cation and anion content, make bentonite backfill a favorable material for use in argillaceous systems (e.g., in borehole and shaft seals) to maintain a constrained water composition (Bradbury and Baeyens

2003; Wersin 2003). The fluid chemistry for the MX-80 bentonite ranges from a Na_2SO_4 water to a $NaCl/Na_2SO_4$ composition with some $CaCl_2$, depending on initial geologic compaction (Bradbury and Baeyens 2003). Although steel canister corrosion is expected to maintain reducing conditions, the addition of Fe⁺² ions is not expected to substantially alter the major water chemistry in the argillaceous system because of Fe-mineral precipitation and the buffering capacities of the clays (Wersin 2003).

As indicated above, the elevated temperatures will shift the solution pH to slightly lower values and may tend to favor solutions that are at the upper end of the concentration ranges that have been observed. The major technical issues relating to elevated temperatures have been evaluated (Johnson et al. 2005). The primary concerns regarding thermal effects are alteration of physical properties from dehydration, and possible illitization at higher temperatures. Significant changes to water composition are not expected from these alteration processes.

2.5.1 Dissolved Radionuclide Solubility Controls

Given the conditions outlined above, bounding estimates can be made for the dissolved concentrations of radionuclides likely to be present once formation fluids come into contact with UNF. Table 2.5-1 identifies likely solubility-limiting phases and provides estimates of dissolved radioelement concentrations *in situ*.

The relatively low solubility of UO₂ (uraninite) under reducing conditions would favor stabilization of used fuel rods. Dissolution would occur at conditions close to equilibrium with uraninite. Because uraninite is the stable uranium phase, negligible oxidative degradation of the waste form would be expected. For example, a natural analogue study of uranium fixation in a Tertiary argillite found that uraninite was the principal secondary uranium phase formed (with less abundant U-phosphate and U-phosphosulfate phases; Havlova et al. 2006). When contacted by water, fuel rods would have diminished thermodynamic drive to dissolve, thus slowing the matrix release of actinides and fission products. Yet even if fuel rods were to instantly degrade to the thermodynamically stable actinide oxides, each of these actinide phases has low solubility that would limit contributions to the source term from the isotopes of Am, Ac, Cm, Np, Pa, Pu, Tc, and Th. A more conservative calculation would use the solubilities of amorphous and/or hydrated phases to bound radionuclide release. Experimental identification of the phase(s) that would control long-term solubility for the individual radionuclides is an important target for future research.

It is less clear whether iodine, radium, and strontium would form solubility-limiting solids. If clay/shale fluids contained appreciable sulfate, $SrSO_4$ and $RaSO_4$ might form to limit dissolved Sr and Ra levels. These phases would be more likely to form in the more sulfate-rich solutions found in some bentonite backfill materials (Bradbury and Baeyens 2003). Dissolved carbonate might also lead to the formation of $SrCO_3$. Low values for dissolved Ra concentration $(2 \times 10^{-11} \text{ M})$ were based on a solid solution model for Ra within barium sulfate (Schwyn and Wersin 2004) considering solutions likely to form in bentonite backfill, for the Swiss repository concept in the Opalinus clay. In that study, dissolved Sr was limited to $2 \times 10^{-5} \text{ M}$. There are possible solid solution phases that could incorporate Sr, similar to Ra, such as calcite and barite. Kinetically limited reduction of Se by FeS₂ or possibly organic matter is proposed as a solubility-limiting mechanism (Maes et al. 2004). Radioiodine should be reduced to highly soluble iodide

given sufficient electron donors from steel waste containers and organics in the clay/shale. No limiting concentrations are set for I, Sr, and Ra in Table 2.5-1. These radioelements would be controlled by their inventories and the slow dissolution rates of the waste forms, for example the matrix UO_2 grains of the spent fuel.

Radioelement	Solubility-Limiting Phase	^A Dissolved Concentration (moles/L)	Notes
Am	AmOH(CO ₃)	1×10^{-6}	
Ac	(see note)	1 × 10 ⁻⁶	Am solubility is used as proxy for chemically similar Ac.
С	(none)	(none)	Likely limited by calcite growth
Cm	(see note)	1×10^{-6}	Am solubility is used as proxy for chemically similar Cm.
Cs	(none)	(none)	No solubility limiting phase
I	(none)	(none)	No solubility limiting phase
Np	NpO ₂	6×10^{-12}	
Pa	PaO ₂	6×10^{-12}	Np solubility is used as proxy for chemically similar Pa.
Pu	Pu(OH) ₄	5×10^{-6}	
Ra	RaSO ₄	(none)	Possible solid solution with BaSO ₄
Se	Possibly Se ⁰	$3.0 imes 10^{-9}$	Kinetic reduction from oxyanions
Sr	Possibly SrCO ₃ , SrSO ₄	(none)	Possible solid solution
Тс	TcO₂	3×10^{-31}	
Th	Th(OH) ₄	$6.0 imes 10^{-8}$	
U	UO ₂	$1.0 imes 10^{-9}$	

Table 2.5-1. Radionuclide Solubilities at T = 100°C, pH 7

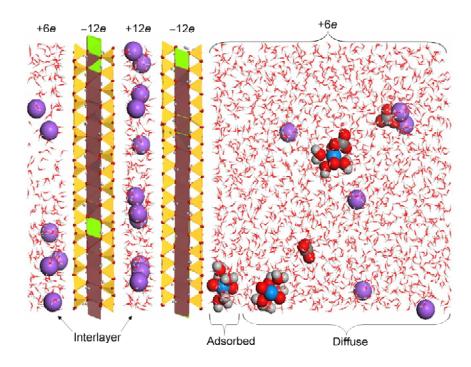
^A Calculated using the PHREEQC code version 2.12.03 and the thermo.com.V8.R6.230 database from Lawrence Livermore National Laboratory, except for the 25°C TcO₂ solubility product and enthalpy, which came from the R5 version of the Yucca Mountain Project thermodynamic database. The solution assumed 50 mmol S, 50 mmol bicarbonate, and calcite saturation.

2.5.2 Radionuclide Sorption

Performance assessment models of proposed and existing geologic repositories are commonly limited by the lack of definitive experimental data describing the adsorption of waste species onto the important mineral surfaces in the natural system. Adsorption data obtained from laboratory-scale batch and column experiments, and especially field determinations, can be difficult to interpret due to the highly complex nature of flow in mixed-phase porous media and the interactions of fluids with complex mineral surfaces. Adsorption data from the scientific literature are generally restricted to specific ranges of temperature, solution composition, pH, and ionic strength, and therefore have limited applicability to conditions expected along transport pathways from a repository. Clay/shale media have great potential for radionuclide sorption, which could be readily demonstrated and enhanced based on site-specific, repository-relevant experimentation.

The last decade has seen the use of computational chemistry methods to improve the understanding of clay minerals and associated phenomena. In particular, molecular dynamics simulations have begun to provide critical adsorption data associated with the binding of various cations onto the surfaces of important clay minerals. Molecular modeling efforts have demonstrated that structures, swelling, adsorption, and related processes of clay minerals can be accurately predicted. Progress in the theoretical determination of adsorption is due in part to the improvement in simulation methods and the development of improved energy force fields (e.g., Cygan et al. 2004) to better model water–mineral systems.

For example, recent studies by Greathouse and Cygan (2005; 2006) demonstrate the use of largescale molecular dynamics simulations to assess the variation of uranyl cation adsorption onto the external surface of various 2:1 dioctahedral clays. The simulations provide atomistic detail to help explain experimental trends in uranyl adsorption onto natural media containing smectite clays (Figure 2.5-1). Adsorption can be evaluated as a function of clay surface, clay layer charge, solution composition, and ionic strength. Atomic density profiles derived from the molecular dynamics trajectories have been used to obtain k_d values and related adsorption parameters that can be used in performance assessment. Such values can be used in conjunction with, or as a supplement/alternative to, compilations of k_d values from sorption experiments.



NOTE: Sodium ions (purple spheres) and carbonate ions (gray and red spheres) form various associated complexes. Water molecules are highlighted as red and gray spheres when associated with uranyl.

Figure 2.5-1. Snapshot from a Large-Scale Molecular Dynamics Simulation of the Adsorption of Hydrated Uranyl (blue and red spheres) onto the Basal Surface of Sodium Montmorillonite Used to Predict the Partitioning of Radionuclides in the Environment

Table 2.5-2 provides a compilation of k_d values for radioelement sorption onto sediments and clays. Distribution coefficients tend to lump together multiple equilibrium and kinetic reactions and are specific to the conditions under which they were measured (e.g., pH, ionic strength,

temperature, fluid-to-rock ratio, among others). Therefore, they provide only an approximate representation of the potential for contaminant retardation. Nevertheless, k_d values are useful in examining controls on radioelement transport. Ultimately, the molecular-level approach described above would be used to update and extend values such as those shown in Table 2.5-2.

Element	k d sediment	K d bentonite
Am, ^a Ac, ^a Cm	100 to 100,000	300 to 29,400
С	0 to 2000	5
Cs	10 to 10,000	120 to 1000
Np, ^a Pa	10 to 1000	30 to 1000
Pu	300 to 100,000	150 to 16,800
[⊳] Ra	5 to 3000	50 to 3000
Se	0.1 to 100	4 to 30
Sr	5 to 3000	50 to 3000
°Tc	0 to 1000	0 to 250
Th	800 to 60,000	63 to 23,500
U	20 to 1700	90 to 1000
I	0 to 100	0 to 13

Table 2.5-2. Sediment and Clay k_d Values (mL/g)

^a k_d values for Ac and Cm are set equal to those of chemically similar Am. k_d

values for Pa are set equal to those of chemically similar Np.

^b k_d values for Ra were set equal to those of chemically similar Sr.

^c Tc k_d values for reducing conditions will likely be much greater than the zero values listed here, which were measured under more oxidizing conditions.

NOTE: All values are from the review of McKinley and Scholtis (1993). Values less than one were rounded down to zero.

Elements with k_d values of 0 (e.g., iodine) do not sorb and will therefore move at the velocity of the fluids that carry them. Elements with k_d values of 10 or greater will move at less than 1% of the velocity of deep fluids. Schwyn and Wersin (2004) reported substantially higher values for sorption coefficients for the Opalinus clay and bentonite backfill, respectively, for Np/Pa (50,000/5000 mL/g; 60,000/5000 mL/g), Tc (50,000 mL/g; 60,000 mL/g), and U (20,000 mL/g; 40,000 mL/g). For Tc, these reflect the more reducing conditions in these fluids compared to the oxidizing conditions represented in the experimental values in Table 2.5-2. Regardless, Table 2.5-2 emphasizes that sorption will sharply limit the transport of most radionuclides from clays and shales. The two exceptions are isotopes of iodine and carbon, namely ¹²⁹I and ¹⁴C. Although ¹⁴C does not sorb because it is primarily anionic in solution over the relevant pH range, it would be substantially decay before release to the biosphere.

2.5.3 Dispersion and Molecular Diffusion

In principle the k_d values in Table 2.5-2 can be used to calculate effective diffusion coefficients for individual radionuclides in clays. The modeled diffusive flux of contaminants (*J*, in units of mol/m²-sec) lumps together physical dispersion and chemical transport in response to a concentration gradient. Sorption onto porous media that occurs simultaneously must be accounted for as well. The one-dimensional diffusive flux is the product of the effective diffusion coefficient for the solute, D_e (m²/sec), and the solute concentration gradient,

$$J = \theta D_e \frac{\partial C}{\partial x}$$
(Eq. 2.5-1)

 D_e accounts for physical dispersion and the chemical characteristics of the diffusing species. The two processes are separated out in the calculation of diffusive flux in porous media (no sorption):

$$J = -\theta \frac{\delta}{\tau^2} D_w \frac{\partial C_p}{\partial x}$$
(Eq. 2.5-2)

where θ is the porosity accessed by diffusing species; δ is constrictivity; τ is tortuosity; D_w is the diffusivity of the radionuclide in aqueous solution (m²/sec); and c_p is its concentration in the porewater. The first three variables account for physical dispersion, the last two for chemical diffusion. To include sorption, the equation becomes:

$$J = -\theta \frac{\delta}{\tau^2} D_w \frac{\phi}{\left[\theta + (1-\theta)\rho k_d\right]} \frac{\partial C_p}{\partial x}$$
(Eq. 2.5-3)

where ρ is density (g/mL). For a non-sorbing tracer with $k_d = 0$, the equation above reduces to the case of simple diffusion.

In principle one could calculate radionuclide diffusion fluxes from measured k_d values, the molecular diffusion coefficient of the particular radionuclides and the porosity, constrictivity, density, and tortuosity of the clay. In practice, each of the parameters is assumed to remain constant and the parameter $\theta \frac{\delta}{\tau^2} D_w \frac{\phi}{[\theta + (1-\theta)\rho k_d]}$ is measured experimentally and given in terms of the apparent diffusion coefficient D_a (m²/sec). D_a is related to the effective diffusion coefficient D_e by: $D_a = \frac{D_e}{\theta + (1-\theta)\rho k_d}$ with $D_e = \theta \frac{\delta}{\tau^2} D_w$.

Representative measured values of D_a in bentonite (representing clay/shale media and backfill/buffer or sealing materials) are:

Non-sorbing, uncharged species (tritium): 10^{-9} m²/sec (Bradbury and Baeyens 2002) Anions such as iodide: 3 to 7×10^{-11} m²/sec (Lee et al. 1994) Moderately sorbing cations such as neptunyl and Cs⁺: 10^{-12} to 6×10^{-11} m²/sec, depending on the dry density of the bentonite (e.g., Bradbury and Baeyens 2002) More strongly sorbing cations: 10^{-12} m²/s.

 D_a values used for the generic performance analysis in this report are:

I, C, Tc: 10^{-10} m²/sec Cs, Np, U, Np, Pa: 10^{-11} m²/sec Am, Ac, Cm, Pu, Ra, Se, Sr, Th: 10^{-12} m²/sec.

3. SCENARIO ANALYSIS

Consistent with the approach taken in 40 CFR 197, it is assumed that the mean annual dose from a repository in clay/shale will include probability-weighted consequences of releases due to all significant FEPs, and will account for uncertainty associated with those FEPs. As described below in Section 3.1, a FEP screening approach similar to that taken for both Yucca Mountain and WIPP is adopted to identify the significant FEPs that should be included in the performance analysis. Section 3.2 describes how FEPs that are identified as being significant to performance are combined into the scenario analyzed in Section 4.

3.1 Identification of Relevant Features, Events, and Processes

The mechanics of constructing scenarios consists of five basic steps (DOE 2008; DOE 1996; Swift et al. 1999): (1) identify a list of FEPs potentially relevant to long-term performance of the disposal system; (2) select FEPs to include and those to omit in PA; (3) construct scenarios from retained FEPs for further screening or analysis; (4) select scenarios to include in PA; and (5) implement and analyze the scenarios in the PA in association with modelers as described in Section 4.

Various programs in the U.S. and elsewhere have compiled exhaustive lists of FEPs for mined geologic disposal that should be evaluated for potential relevance. For this analysis, a preliminary FEP list developed by the Used Fuel Disposition (UFD) Program for Nuclear Energy Office of DOE was used (see Appendix B, Table B-1). The UFD FEP list generalizes the FEP list for the Yucca Mountain license application (DOE 2008), which in turn, was based on FEP list for the WIPP Compliance Certification Application (DOE 1996; DOE 2004; DOE 2009) and the FEP list for the Nuclear Energy Agency (NEA) of the Organisation for Economic Co-Operation and Development (OECD). The UFD FEP list was also compared to the NEA FEP catalogue specifically for argillaceous media (NEA 2003) to examine FEPs that may be unique to disposal in clay/shale.

As noted above, once potentially relevant FEPs for performance of a repository in clay/shale have been identified, they must be evaluated against screening criteria provided in U.S. regulations. Specifically, EPA standard 40 CFR 197 states that FEPs that have an annual probability of occurrence less than one chance in 10^8 in the first 10,000 years after closure may be excluded from the analysis. Features, events, and processes that have higher probabilities, but do not significantly change the results of long-term performance assessments, may also be omitted from the analysis (40 CFR 197.36(a)(1)). In addition, some potentially relevant FEPs are screened from further consideration because they are inconsistent with specific aspects of the regulatory requirements. For example, existing regulations for WIPP and Yucca Mountain indicate that performance assessments should not include consequences of deliberate human acts of sabotage or disruption in the far future.

Each of the 216 UFD FEPs has been considered (screened) for potential relevance to disposal in clay/shale formations. Table B-1 in Appendix B summarizes the screening decisions for each FEP (whether a FEP is likely to need to be included in or excluded from a full performance assessment for a clay/shale repository) and also includes a qualitative estimate of the level of effort likely to be required to provide a robust basis for the screening of the FEP.

3.2 Scenario Selection

In evaluating UFD FEPs for the clay/shale repository performance analysis, the following assumptions are made consistent with performance assessments for Yucca Mountain (10 CFR Part 63):

- The water well use is consistent with the lifestyle of a person in an arid environment as occurs near Yucca Mountain, Nevada. All biosphere pathways associated with contaminated well water use (e.g., irrigation, crops, livestock, drinking, etc.) are included.
- The mixing with uncontaminated water at the withdrawal well is consistent with a community pumping 3,000 acre-feet per year for mixed domestic and agricultural use.

For the purposes of this analysis, the following assumptions are made that go beyond the regulatory requirements for Yucca Mountain performance assessment, and the FEP screening decisions of Appendix B:

- Biosphere exposure is assumed to occur via a contaminated groundwater well immediately above the repository host formation. There is no transport pathway vertically or horizontally in the aquifer above the repository host rock that includes sorption.
- No credit is taken for the engineered barrier system (i.e., corrosion rate of waste package or degradation rate of the waste form as barriers) that delays or attenuates releases. Therefore, all FEPs related to the performance of waste package and waste form as flow and transport barriers are excluded from the analysis.
- The repository is placed in a low permeability clay/shale with a small hydraulic gradient.
- The repository is placed in the saturated zone, in clay/shale containing organic matter or minerals such as pyrite, such that chemically reducing conditions limit the rate of waste form degradation and retard radionuclide transport.
- No performance credit is taken for radionuclide attenuation in the EDZ; instead, the EDZ extent is subtracted from the distance from the repository to the overlying aquifer.

From consideration of the FEPs that have a preliminary screening of "included" in Appendix B and additional conditions listed above, radionuclides emplaced in a clay/shale repository in the saturated zone might reach the biosphere along two principal paths for a nominal scenario: (1) through the short-lived EDZ and through or around shaft seals; (2) outward through the host clay/shale formation. Disruption of the repository through human intrusion is a second scenario. A more complete screening of the FEPs may identify additional scenarios of interest, and may also show that some aspects of the chosen scenarios do not need further analysis. Also, note:

• Though part of the nominal scenario developed below, release via transport through the repository backfill or the short-lived EDZ, and through or around shaft seals, is not considered in the PA in Section 4.

• Though a scenario is developed below, release from a human intrusion disruptive event is not considered in the PA in Section 4.

Nominal Scenario, Pathway 1: Advective transport through the EDZ and shaft seals.

Hydrologic flow through the repository and up the shafts transports radionuclides to a shallow aquifer from which they are pumped to the biosphere – This pathway scenario requires sufficiently high permeability within the repository, the EDZ, and seals, and a sustained upward gradient in hydrologic potential. An upward gradient in hydrologic potential could result from: (1) ambient hydrologic conditions, (2) thermal pressurization of fluid within the waste disposal zone from waste heat, (3) buoyancy of heated fluid within the waste disposal zone, or (4) thermo-chemical reactions that release water and/or gases within the waste disposal zone. Only ambient hydrologic conditions would operate over long time scales; the thermally driven mechanisms would cease within a few hundred years. Self-sealing of the EDZ, and eventual consolidation of clay components in the shaft and emplacement borehole seals, would limit such a high permeability pathway. Finally, advection along the EDZ and up the access shafts requires a source of water inflow from the clay/shale with sufficient strength to flood the repository, and with greater hydraulic head than the overlying aquifer (to maintain flow). Such conditions are unlikely if other conditions for siting in clay/shale media are met (Section 1.2).

Nominal Scenario, Pathway 2: Diffusive transport in host clay/shale. *Diffusion coupled with a small hydraulic gradient, transports radionuclides upward from the repository, through the clay/shale host rock, to a shallow aquifer from which they are pumped to the biosphere –* Radionuclide transport would occur primarily because of diffusion, in the nominal scenario. Advective flow (under realistic hydraulic gradients) is insignificant during the repository performance period, given the low permeability of clay/shale media. The reducing environment typical for clays and shales would limit radionuclide solubility, thus limiting mobility. Also, the minerals present in clay/shale formations readily sorb many radionuclides, further attenuating releases. Finally, because of the long-transport times, radioactive decay is an important aspect.

Disruptive, Human Intrusion Scenario: Advective transport up one or more unsealed boreholes drilled in the future after repository closure. *A borehole for hydrocarbon exploration is drilled through the repository and later abandoned; a vertical hydrologic gradient transports radionuclides to a shallow aquifer from which they are pumped to the biosphere. This is a stylized calculation specified by 40 CFR 197. Implementation for a clay/shale repository would be inherently similar to the human intrusion scenario in the performance assessment for the WIPP (DOE 2009) and is not analyzed in this report.*

4. PERFORMANCE ANALYSIS

Based on the scenario analysis described in Section 3, a generic performance analysis of a repository situated in a clay/shale formation was performed. The conceptual model, based on the nominal scenario Pathway 2 (Section 3.2), is as follows:

- The assumed repository layout is the "USA" design shown in Figure 2.1-1, consisting of 0.7-m diameter emplacement boreholes drilled horizontally from a 5-m diameter horizontal access tunnel. The emplacement boreholes (i.e., the waste disposal zone) are at a depth of 450 m below the land surface. The overlying geologic units, from the repository to the ground surface, consist of clay/shale (150 m), a sandstone aquifer (100 m), and sediments (200 m).
- Each waste package contains a single PWR assembly (equivalent to approximately 0.4 MTHM) in a 5-m-long package, and is emplaced horizontally in an emplacement borehole. As many as six such packages would be emplaced in each 40-m-long emplacement borehole. The repository would include 200,000 waste packages distributed in a horizontal array (i.e., a single emplacement level).
- The initial radionuclide inventory is consistent with Appendix A (CSNF/PWR) from Brady et al. (2009). The effects of radionuclide ingrowth are accounted for in the analysis using a bounding approximation. The choice of UNF (PWR) rather than HLW for this assessment is conservative with respect to dose. The waste loading (expressed as equivalent MTHM per meter of emplacement borehole) is approximately the same for HLW and UNF, but the UNF contains a greater number of radionuclides, especially actinides, that could contribute to dose.
- The radionuclide source term (dissolved radionuclide concentrations in the waste disposal zone) is limited by thermal-chemical conditions (based on radionuclide solubilities in Table 2.5-1). No credit is taken for delayed or attenuated rates of degradation of the waste package or waste forms. Both are considered to degrade instantaneously, so that the full inventory is available in soluble form (subject to concentration limits) immediately after repository closure. Source depletion is implemented by zeroing the contaminant concentrations in the emplacement borehole, after the full inventory has diffused or advected into the host rock.
- Radionuclide source term concentrations are further limited for U, Am, Pu, Th, and Ra, each of which has more than one isotope present in the waste form. Assuming congruent release of the isotopes from the waste form, the limiting concentration for each isotope is limited to the elemental solubility limit multiplied by the mole fraction. This treatment is consistent with the assumption of instantaneous waste form degradation, and does not affect the fission product isotopes and ²³⁷Np that dominate the estimated dose for 1,000,000 years.
- Advective groundwater flow through the clay/shale host rock is negligible. The clay/shale permeability is assigned a value of 10^{-19} m² (corresponding to hydraulic conductivity of approximately 10^{-12} m/sec; Table 1-2), and the clay/shale transport porosity is assigned a

value of 10%. The upward hydraulic gradient is assumed to be 0.001, so that the resulting upward pore velocity is approximately 3.15×10^{-7} m/yr. The corresponding advective travel time (unretarded) through the 150 m thick clay unit is greater than 100 million years, which is consistent with the long-term stability of natural hydrogeochemical conditions in clay/shale formations. Sensitivity analysis shows that the predicted dose at 1,000,000 years is relatively insensitive to the hydraulic gradient, as long as the advective pore velocity is less than approximately 10^{-4} m/yr.

- Gas generated by chemical and microbial activity in the repository could produce a • driving pressure for advective transport locally, and would be evaluated for inclusion in a more refined PA (Appendix B; FEP 2.2.12.02). However, gas formation will be transient, the effects of gas pressure excursions will readily dissipate, and the performance results presented here are relatively insensitive to the hydraulic gradient; therefore, gas generation is excluded.
- Thermal-hydrologic-mechanical effects (Section 2.3) are considered short-term and negligible beyond the extent of the EDZ. Within the EDZ the effects are limited to one order-of-magnitude increase in hydraulic conductivity. The EDZ is limited in extent to a few meters at most (Section 2.3.2) and is not considered in the transport path length.
- Radionuclide transport from the repository upward for a distance of 150 m through the clay/shale host rock is dominated by aqueous diffusion and sorption, using transport parameters described in Section 2.5. Advection is a minor contribution. Colloids are not readily transported in clay/shale media (Appendix B; FEP 2.2.09.59).
- Radionuclides that reach the upper boundary of the clay/shale are assumed to mix with • water in a sandstone aquifer, which is pumped at a prescribed rate (e.g., 3,000 acre-feet per year). The sandstone aquifer is assumed to directly overlay the emplaced waste. No credit is taken for sorption or decay within the aquifer or for any horizontal transport time that would be required to reach a non-overlying aquifer.
- Dose to a hypothetical person living near the withdrawal well is based on biosphere dose • conversion factors (BDCFs) consistent with the lifestyle of the Yucca Mountain reasonably maximally exposed individual (RMEI), as described by 40 CFR 197.

The conceptual model was implemented numerically in a Microsoft Excel spreadsheet. The numerical solution was used to calculate source concentrations and one-dimensional radionuclide transport for 29 selected radionuclides:

- Actinium series: ²⁴³Am, ²³⁹Pu, ²³⁵U, ²³¹Pa, ²²⁷Ac
 Uranium series: ²⁴²Pu, ²³⁸U, ²³⁸Pu, ²³⁴U, ²³⁰Th, ²²⁶Ra
 Neptunium series: ²⁴⁵Cm, ²⁴¹Pu, ²⁴¹Am, ²³⁷Np, ²³³U, ²²⁹Th
- Thorium series: ²⁴⁰Pu, ²³⁶U, ²³²Th, ²²⁸Ra, ²³²U
- Fission and activation products: ${}^{14}C$, ${}^{79}Se$, ${}^{90}Sr$, ${}^{99}Tc$, ${}^{129}I$, ${}^{135}Cs$, ${}^{137}Cs$.

The dose calculation is limited to twelve of these radionuclides that could potentially transport far enough in 1,000,000 years to contribute to dose (239 Pu, 242 Pu, 237 Np, 233 U, 234 U, 236 U, 238 U, 14 C, 79 Se, 99 Tc, 129 I, and 135 Cs).

One-dimensional radionuclide transport through the clay/shale, with sorption and decay, is described by an advection-dispersion model (de Marsily 1986, Equation 10.3.3; Schwartz and Zhang 2003, Equation 23.27):

$$R_{f} \frac{\partial C}{\partial t} = D_{x} \frac{\partial^{2} C}{\partial x^{2}} - v_{x} \frac{\partial C}{\partial x} - R_{f} \lambda C$$
 (Eq. 4-1)

where:

C = dissolved radionuclide concentration (mg/L) $v_x = \text{groundwater pore velocity (m/yr)}$ $D_x = \text{coefficient of hydrodynamic dispersion (m²/yr)}$ $R_f = \text{retardation factor}$ $\lambda = \text{radioactive decay constant (yr⁻¹)}.$

The coefficient of hydrodynamic dispersion captures the effects of mechanical dispersion (described as a Fickian process; Section 2.5.3) and chemical diffusion in the clay/shale:

$$D_x = \alpha_x v_x + \tau \ D_m \tag{Eq. 4-2}$$

where:

 α_x = longitudinal dispersivity (m) D_m = molecular diffusion coefficient (m²/yr) τ = tortuosity

and the molecular diffusion coefficient is related to the effective diffusion coefficient, D_e (m²/yr), as follows:

$$D_e = n \tau D_m \tag{Eq. 4-3}$$

The retardation factor dispersion captures the effects of sorption in the clay/shale:

$$R_f = 1 + \frac{\rho_b k_d}{n} \tag{Eq. 4-4}$$

where:

$$\rho_b$$
 = bulk density of clay/shale (assumed to be 2200 kg/m³)

- k_d = distribution coefficient (mL/g)
- *n* = porosity (assume full liquid saturation).

A one-dimensional analytical solution to Equation 4-1, for an initial condition of C = 0 (at all x) and a constant-source ($C = C_0$) upstream boundary condition, is (de Marsily 1986, Equation 10.3.4; Schwartz and Zhang 2003, Equation 23.36):

$$C(x,t) = \frac{C_0}{2} \left[e^{\frac{xv_x}{2D_x}[I-\Omega]} erfc \left(\frac{x - \frac{v_x}{R_f} t\Omega}{2\sqrt{D_x t/R_f}} \right) + e^{\frac{xv_x}{2D_x}[I+\Omega]} erfc \left(\frac{x + \frac{v_x}{R_f} t\Omega}{2\sqrt{D_x t/R_f}} \right) \right]$$
(Eq. 4-5)

where:

$$\Omega = \sqrt{1 + \frac{4\,\lambda D_x R_f}{v_x^2}}$$

In Equation 4-5, R_f (due to k_d), D_x (due to D_m), and λ are all radionuclide-specific. All other parameters are the same for all radionuclides. An additional radionuclide-specific parameter is the radionuclide or contaminant velocity, v_c (m/yr), which is calculated as follows:

$$v_c = \frac{v_x}{R_f}$$
(Eq. 4-6)

A comparison of the dispersion term (Equation 4-2, first term on right-hand side) and the diffusion term (second term) shows that even for ¹²⁹I, which is nonsorbing and therefore has the fastest contaminant transport rate, the ratio of diffusion to dispersion is greater than 600. This confirms that diffusion is the dominant process.

Equation 4-5 is used to calculate the transport flux (mg/m^2-yr) for each of the 29 radionuclides at the clay/shale interface with the sandstone (x = 150 m) as a function of time, *t* (Figure 4-1). The cross-sectional area for transport is the plan area of host rock containing one waste package, extending between the midpoints to the adjacent emplacement boreholes (i.e., for a 20-m borehole spacing and 5-m waste package length, the transport area is 100 m²). The source concentration is diluted by the ratio of the transport area to the maximum footprint area of the waste package to the transport area is not included in the model, the approach is considered to be conservative with respect to dose because it neglects downward diffusive transport, away from the biosphere.

The source concentration, C_0 , is determined by: (1) calculating a maximum potential concentration based on dissolving the entire initial mass inventory in a PWR assembly into the void volume (i.e., the potential volume of water) of a waste package; and (2) selecting the lesser of the maximum potential concentration and the solubility limits (see Table 2.5-1) as the source concentration. The source concentration is assumed to remain constant for a period of time determined by the initial radionuclide mass and the rate of transport into the host rock, and is then set to zero at the point in simulation time when the initial mass is fully depleted. This approach overestimates the rate of release from the EBS to the host rock, and is therefore

conservative with respect to calculated dose. The concentration is set to zero using superposition, by subtracting a replicate of the solution (Equation 4-5), starting when the source is depleted. Use of superposition with this advection-dispersion solution is consistent with other published applications (de Marsily 1986, p. 270).

Radionuclide concentration profiles in the clay/shale layer are shown for 1,000,000 years (Figure 4-2). By 1,000,000 years, the following radionuclides have reached the aquifer (in order of concentration above 10⁻¹⁰ mg/L): ¹²⁹I, ²³⁸U, ²³⁶U, ⁷⁹Se, ²³⁴U, ²³³U, ¹³⁵Cs, and ²³⁷Np. Only radionuclides with potentially significant concentrations at or near the 150 m boundary at 1,000,000 years are included in the dose calculation (Figure 4-3). Dose is calculated by solving for concentration profiles at many time steps, and integrating the profiles to determine the total radionuclide mass (dissolved and sorbed) in the clay/shale layer, and above the clay/shale layer. The region beyond the clay/shale layer is represented by extending the solution (Equation 4-5) to 10 km. In the conceptual model, the integrated radionuclide mass beyond 150 m is taken up immediately in water pumped from the aquifer, which is a "swept away" boundary condition that does not affect the diffusive flux within the clay/shale layer. This is based on an assumption that the concentration gradient changes slowly across the shale-sandstone boundary.

The corresponding dose to the RMEI, based on the mass fluxes into the sandstone aquifer, is plotted in Figure 4-3 by radionuclide, as a function of time. The doses are well below the current regulatory limit of 100 mrem/yr for 1,000,000 years (Section 1.3); the maximum of the total dose considering all radionuclides included in the analysis is less than approximately 0.01 mrem/yr. This result is for PWR UNF; the dose for HLW would generally be smaller because of the smaller inventory of radionuclides per repository plan area. These results are based on several simplifying assumptions, including: all waste is assumed to instantly degrade and dissolve inside the waste packages; all waste is assumed to be PWR assemblies; unlimited availability of moisture for waste form degradation and transport; no sorption on degraded waste package materials; and no credit is taken for horizontal transport to, or sorption or decay within, the sandstone aquifer. Also, the repository is assumed to be isolated from through-going hydrologic features such as faults or fracture zones that could provide preferential pathways for groundwater or radionuclides. A more refined performance assessment is needed to examine the relative importance of these assumptions. Similarly, other release pathways, such as nominal scenario Pathway 1 (Section 3.2), or the human intrusion scenario, or different repository or source configurations, would also require model refinements.

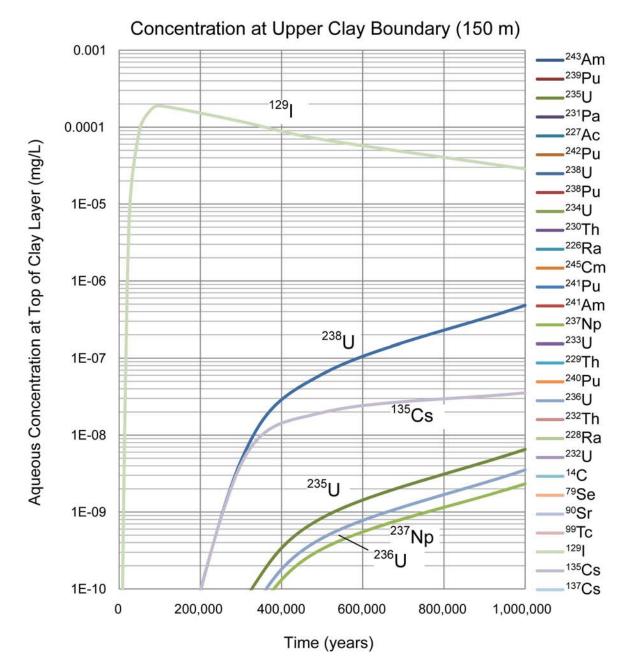
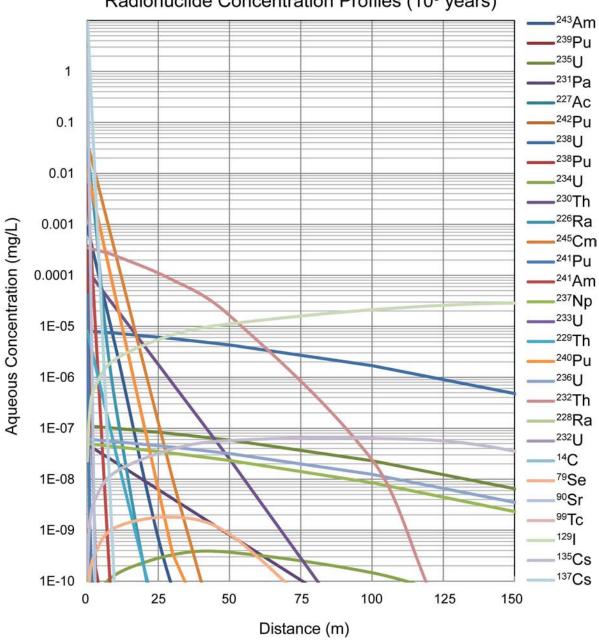


Figure 4-1. Aqueous Radionuclide Concentrations at the Top of the Clay/Shale Layer Overlying a Single Waste Package, as Functions of Time, for 29 Radionuclides



Radionuclide Concentration Profiles (10⁶ years)

Figure 4-2. Concentration Profiles, by Radionuclide, in the Clay/Shale Unit Overlying a Single Waste Package at 1,000,000 Years after Emplacement



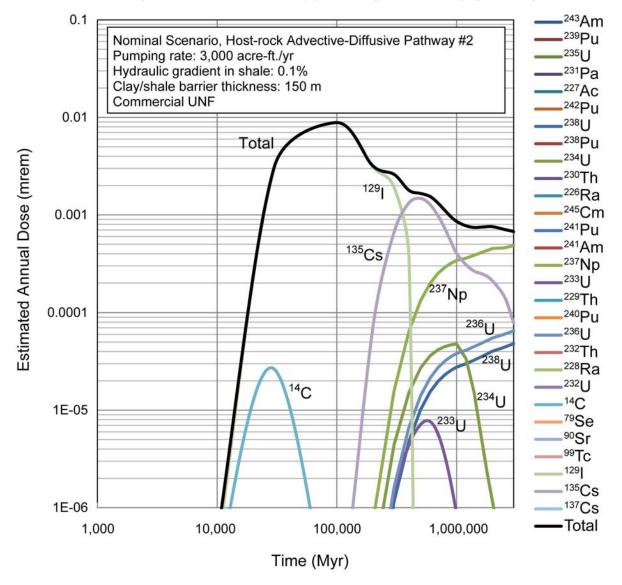


Figure 4-3. Dose Calculation for 200,000 Waste Packages, by Radionuclide (for significant contributors) as Functions of Time

5. SUMMARY AND CONCLUSIONS

This report establishes that the U.S. has vast land areas with clay/shale formations of sufficient thickness and lateral extent to incorporate a nuclear waste repository. International nuclear waste repository programs have advanced the engineering and science of waste disposal in clay/shale media, to provide great confidence that such a repository could be safely constructed, operated, and sealed. The waste isolation performance for a clay/shale repository would readily satisfy expected regulatory performance objectives. Finally, the sophisticated multi-physics modeling techniques used for this analysis are sufficiently advanced to model first-order interplay of the important thermal, hydrological, and chemical processes. This report presents a snapshot view of a clay/shale repository for HLW and UNF that, while generic in nature, casts a favorable light on the potential for successful implementation.

5.1 Summary of Findings

The regulatory requirements will need to be modified to accommodate virtually any new geologic disposal option, including a nuclear waste repository in clay or shale. The suitability of clay/shale media has been established by international repository programs, which have advanced engineering, scientific, and operational concepts. Sections 1 and 2 of this report provide a high-level summary of this progress, and of previous clay/shale investigations in the U.S. From this publicly available information, the framework for evaluating a generic clay/shale repository in the U.S. was developed.

The literature abounds with information on clay behavior, due partly to international repository programs and the persistent collaborative research by the "Clay Club" as referenced extensively in this report. The technical literature is replete with citations of the positive attributes of clay/shale performance as a repository medium:

- Slow fluid movement Low hydraulic conductivity ($\sim 10^{-12}$ m/sec or less) and diffusion-dominated transport.
- **Self-sealing** Clay/shale formations commonly exhibit plastic deformation, so that fractures formed by excavation and heating will close and seal.
- **Reducing chemical conditions** Reducing conditions will maintain waste forms and most radionuclides at very low solubilities. Sorption of many radionuclides onto clays with high specific surface area will also retard transport.

The technical literature was consulted to characterize the repository setting and select material properties, while design information and a concept of operations were based on practices previously adopted by international programs.

The repository geometry, material properties, thermal loading, and other features of this analysis were chosen to represent a plausible repository implementation concept. Further evaluation of tunnel deformation and stability, operational functionality, and the effects of excavation and heating on long-term performance would require development and application of site-specific constitutive models for the clay/shale. Even in this generic assessment, the value of three-

dimensional multi-physics calculations is demonstrated by identifying sensitive aspects of the underground setting. Three-dimensional grids were used to simulate the THM and chemical transport behavior of a repository sited in clay/shale below the water table. Thermal loading was chosen to produce waste package temperatures approaching 100°C, and also to provide bounding calculations. Based on these results, a clay/shale repository could accept all waste from the current inventory for emplacement, with the use of up to 50 years of decay storage for the hottest UNF. Thermal-hydrologic processes considered include saturated and unsaturated liquid flow, evaporation/condensation, and convective heat transport. These processes are limited in low-permeability media, and rapidly subside as the repository cools within a few hundred years. The mechanical results, based on an elastic-perfectly plastic constitutive model, showed inelastic response extending to several opening diameters around the access drift, but more limited plasticity was predicted to occur around the emplacement borehole. This result depends on the constitutive models used to represent the host rock, but is consistent with the repository design concept adopted from international investigations.

A generic performance analysis is presented for a repository situated in a clay/shale formation, using conceptual models and simplifications consistent with the international state of practice. The preliminary generic FEP list from the Used Fuel Disposition (UFD) Program was adopted as a starting point for this analysis. Each of the 216 FEPs on that list was screened for potential relevance to disposal in clay/shale formations (Appendix B). The NEA (2003) FEP catalogue for argillaceous media was also examined. Three basic scenarios were developed whereby radionuclides could be transported to a hypothetical aquifer, from which they would be pumped to the biosphere: (1) short-term, advective transport through the repository openings or the EDZ, and up the shafts; (2) long-term, diffusive transport through the host clay/shale upward from the emplacement boreholes; and (3) a stylized human intrusion scenario. The first scenario is not of interest for this preliminary analysis because of its short-term nature, the likely effectiveness of engineered seals, and the lack of a strong hydraulic pressure gradient to drive water through the repository and up the shafts. The third scenario is also not of interest for this work because it is stylized and only consequences are evaluated. Only the second scenario was considered in the generic performance analysis, using a one-dimensional advective-dispersive model formulation.

Thermal, hydrologic, and geochemical calculations suggest that radionuclides in a clay/shale repository will not migrate far from the disposal horizon. The great majority of radionuclides in the current waste inventory will be thermodynamically stable as solids and will therefore resist migration. Much of the inventory will decay before transport to the biosphere can occur. The calculated dose to the reasonably maximally exposed individual, based on the radionuclide mass flux into a hypothetical overlying sandstone aquifer, is 0.01 mrem/yr or less at 1,000,000 years, which is far below the regulatory annual dose limit of 100 mrem in the current regulations. The performance analysis predicts that the dose at 10,000 years is effectively zero. These results include conservative assumptions such as instantaneously degraded waste packages and waste forms, unlimited availability of moisture for waste form degradation and transport, no sorption on degraded waste package materials, etc. A further refined performance assessment would be required to examine these assumptions.

Findings of this research are summarized as follows:

- 1. Many areas of the conterminous U.S. have positive characteristics for hosting a geologic repository for HLW and UNF.
- 2. International repository programs have advanced repository science for clay/shale media, and have much to offer if the U.S. resumes investigations for disposal in clay/shale.
- 3. Clay mineralogy and chemistry combine to limit radionuclide transport through the influence of low permeability, chemically reducing environments, and sorption.
- 4. Multi-physics modeling is well advanced to exploit massively parallel computational hardware for simulation of coupled THMC processes. Our ability to predict coupled behavior over long time spans with new computational approaches adds confidence to dose projections. Laboratory and field test parameters are needed to validate and improve the models.
- 5. The clay/shale repository concept will effectively isolate HLW and UNF of all the types that currently exist in the U.S. inventory, considering thermal output, radiological characteristics, and transport to the biosphere.
- 6. Generic performance analysis for a clay/shale repository exhibits excellent performance against existing regulatory standards.
- 7. Experience with seal systems for the WIPP repository would provide significant support to design, construction, testing, and performance assessment for a clay/shale repository.

These findings lead to the conclusion that clay/shale media are highly viable to host repositories for HLW and UNF in the United States.

5.2 Recommendations for Additional Work

Technical studies of shale for repository purposes were engaged in the U.S. for a number of years, ending in the 1980s with implementation of the NWPA and passage of the NWPA Amendments. These historical studies provide useful support for the current report. The actual experimental work was limited, however, and has been surpassed by new experimental and modeling approaches that have been developed by the scientific community in the intervening 30 years. These new methods can provide far greater precision in site characterization, repository design, and performance assessment. The new tools should be deployed in conjunction with an underground test facility, and with strengthened technical exchanges with other nations already committed to developing repositories in clay/shale media.

An underground research laboratory is needed to calibrate and validate models used in design, operation, and performance, and to build confidence by testing alternative models. Cooperation with clay/shale programs in Europe will provide more complete overall technical analysis of the clay/shale disposal option. One of the benefits gained from repository science development over the past 30 years is improved understanding of FEPs that are important to performance. A comprehensive evaluation of potentially relevant FEPs for disposal in clay/shale media is an

early goal, beginning with the preliminary list identified in Appendix B and expanding that list as appropriate. Screening of that FEP list, and limited, iterative performance assessment analyses, would then be used to focus site characterization and testing on important areas. Future performance assessment modeling should consider all relevant release scenarios and transport pathways based on FEP analyses, rather than focusing only on the scenarios considered in this report.

Basic research and development is also needed to support clay/shale repository science. Further investigations could build a technical database that would support the evaluation of volunteer sites. A technical database would support evaluation of the acceptability of proposed repository host geologic media and siting. The THMC responses of clay/shale media are more complex than for salt, tuff, or granite. This complexity can be mitigated to some extent by maintaining sub-boiling (less than 100°C) temperatures, but research needs include measurement of material properties for multi-physics representation of repository performance. Validation of multi-physics predictions depends on full-scale thermal-hydrologic-mechanical field testing in representative clay/shale media. As confidence in multi-physics models increases, they could be used in a science-based approach to evaluate design alternatives, and to predict the outcomes from pilot-scale field tests. International experience has shown that full-scale demonstration of disposal ("proof-of-principle") is needed to build confidence in the disposal concept of operations, and predictions of long-term performance.

Clay/shale formations in the U.S. provide a viable alternative disposal pathway for all types of HLW and UNF, in the nation's portfolio of nuclear fuel cycle options.

6. REFERENCES

American Concrete Institute (ACI) "Building Code Requirements for Reinforced Concrete (ACI 318-77)", August 1978, ACI, Box 19150, Redford Station, Detroit MI.

ANDRA (Agence nationale pour la gestion des déchets radioactifs) 2005. *Dossier 2005 Argile: Evaluation of the feasibility of a geological repository in an argillaceous formation -Meuse/Haute-Marne site*. http://www.andra.fr.

Arnould, M. 2006. Discontinuity networks in mudstones: a geological approach. Implications for radioactive wastes isolation in deep geological formations in Belgium, France, Switzerland. *Bull. Eng. Geol. Environ.* 65:413–422.

Bates, R.L. and J.A. Jackson, eds. 1980. *Glossary of Geology*, 2nd Ed. American Geological Institute, Falls Church, VA. 788 p.

Bernier, F., X. L. Li, W. Bastiaens, L. Ortiz, M. Van Geet, L. Wouters, B. Frieg, P. Blümling, J. Desrues, G. Viaggiani, C. Coll, S. Chanchole, V. De Greef, R. Hamza, L. Malinsky, A. Vervoort, Y. Vanbrabant, B. Debecker, J. Verstraelen, A. Govaerts, M. Wevers, V. Labiouse, S. Escoffier, J.-F. Mathier, L. Gastaldo, and Ch. Bühler 2007. Fractures and self-healing within the excavation disturbed zone in clays (SELFRAC). European Commission EURATOM Report EUR 22585.

Blümling, P., F. Bernier, P. Lebon, and C. Derek Martin 2007. The excavation-damaged zone in clay formations – time-dependent behaviour and influence on performance assessment. *Physics and Chemistry of the Earth, Parts A/B/C. V.32.* Issues 8-14. pp. 588-599.

Boisson, J.Y. 2005. *Clay club catalogue of characteristics of argillaceous rocks*. Organisation for Economic Co-Operation and Development/Nuclear Energy Agency. Report No. NEA-4436.

Bowles, J.E. 1976. Foundation Analysis and Design, 1976, McGraw-Hill, NY, NY.

Bradbury, M.H. and B. Baeyens 2002. A comparison of apparent diffusion coefficients measured in compacted Kunigel V1 bentonite with those calculated from batch sorption measurements and De (HTO) data: A case study for Cs(I), Ni(II), Sm(III), Am(III), Zr(IV) and Np(V). NAGRA.

Bradbury, M.H., and B. Baeyens 2003. Porewater chemistry in compacted re-saturated MX-80 bentonite. *Journal of Contaminant Hydrology*, 61, 329-338.

Brady, P.V., B.W. Arnold, G.A. Freeze, P. N. Swift, S. J. Bauer, J. L. Kanney, R. P. Rechard, and J. S. Stein 2009. *Deep borehole disposal of high-level radioactive waste*. SAND2009-4401, Sandia National Laboratories, Albuquerque, NM.

Carter, L.J. 1987. Nuclear imperatives and public trust: dealing with radioactive waste. Washington, DC: Resources for the Future; Baltimore, MD: John Hopkins University Press.

Colglazier, E.W. and R.B. Langum 1988. Policy conflicts in the process for siting nuclear waste repositories. *Ann. Rev. Energy*, 13:317-357.

Corkum, A.G. and C.D. Martin 2007a. "Modeling a mine-by test at the Mont Terri rock laboratory." Switzerland. *Intl. J. Rock Mech. & Min. Sci.* 44:846-859.

Corkum, A.G. and C.D. Martin 2007b. "The mechanical behavior of weak mudstone (Opalinus Clay) at low stresses." *Intl. J. Rock Mech. & Min. Sci.* 44:196-209.

Cygan, R.T., J.J. Liang, and A.G. Kalinichev 2004. "Molecular models of hydroxide, oxyhydroxide, and clay phases and the development of a general force field." *Journal of Physical Chemistry B*, 108(4), 1255-1266.

de Marsily, G. 1986. *Quantitative Hydrogeology: Groundwater Hydrology for Engineers*. San Diego, California: Academic Press.

DOE 1996. Title 40 CFR Part 191 *Compliance Certification Application for the Waste Isolation Pilot Plant*. DOE/CAO-1996-2184. Carlsbad, NM: DOE Carlsbad Area Office.

DOE 2004. Title 40 CFR Part 191 *Compliance Recertification Application for the Waste Isolation Pilot Plant*. DOE/WIPP 2004-3231. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Field Office.

DOE 2008. *Yucca Mountain Repository Safety Analysis Report*. DOE/RW-0573. NV: U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

DOE 2009. 2009 WIPP Compliance Recertification Application. DOE/WIPP 2009-3424. Carlsbad, NM: U.S. Department of Energy, Waste Isolation Pilot Plant, Carlsbad Field Office.

Edwards, H.C. 2002. *SIERRA Framework Version 3: Core Services Theory and Design*. SAND2002-3616, Sandia National Laboratories, Albuquerque, NM.

Gens, A., J. Vaunat, B. Garitte, and Y. Wileveau 2007. "In situ behavior of a stiff layered clay subject to thermal loading: observations and interpretation." *Géotechnique*, **57**, No. 2, 207-228.

Gonzales, S. and K.S. Johnson, 1984. *Shale and other argillaceous strata in the United States*. Oak Ridge National Laboratory. ORNL/Sub/84-64794/1.

Greathouse, J.A. and R.T. Cygan 2005. "Molecular dynamics simulation of uranyl(VI) adsorption equilibria onto an external montmorillonite surface." *Physical Chemistry Chemical Physics*, 7(20), 3580-3586.

Greathouse, J.A. and R.T. Cygan 2006. "Water structure and aqueous uranyl(VI) adsorption equilibria onto external surfaces of beidellite, montmorillonite, and pyrophyllite: Results from molecular simulations." *Environmental Science and Technology*, 40(12), 3865-3871.

Hansen, F.D. and T.J. Vogt, 1987. *Thermomechanical properties of selected shales*. ORNL/Sub/85-97343/2, Oak Ridge National Laboratory.

Hansen, F.D. and M.K. Knowles 2000. *Design and analysis of a shaft seal system for the Waste Isolation Pilot Plant*. Reliability Engineering and System Safety 69.

Hansen, F.D. 2003. *The Disturbed Rock Zone at the Waste Isolation Pilot Plant*. SAND2003-3407, Sandia National Laboratories, Albuquerque NM.

Havlova, V., A. Laciok, D. Volpalka, and M. Andrlik 2006. "Goechemical study of uranium mobility in Tertiary argillaceous system at Ruprechtov site, Czech Republic." Czechoslovak *Journal of Physics*, 56, Suppl. D., D81-D86.

Holland, J.F. "GSR Analysis Thermo-Mechanical Analysis description," unpublished Sandia National Laboratories internal memo to Daniel Clayton, 6711, October 2008.

IAEA (International Atomic Energy Agency), 2006. *Geological Disposal of Radioactive Waste*. Safety Requirements No. WS-R-4. Vienna, Austria: International Atomic Energy Agency.

ICRP (International Commission on Radiological Protection), 1997. "ICRP Publication 77: Radiological Protection Policy for the Disposal of Radioactive Waste." *Annals of the ICRP*, **27**(Supplement 1997).

Jia, Y., H.B. Bian, G. Duveau, K. Su, and J.F. Shao, 2009. "Numerical modeling of *in situ* behaviour of the Callovo–Oxfordian argillite subjected to the thermal loading." *Engineering Geology*. V.109. Issue 3-4. pp. 262-272.

Jobmann, M. and M. Polster 2007. "The response of Opalinus clay do to heating: A combined analysis of *in situ* measurements, laboratory investigations, and numerical calculations." *Physics and Chemistry of the Earth*, V.32. Issues 8-14. pp. 929-936.

Johnson, L., P. Blümling, A. Gautschi, and P. Wersin 2005. "Development of thermal criteria for a SF/HLW repository" in: *Opalinus clay. Engineered Barrier Systems (EBS) in the Context of the Entire Safety Case, Process Issues.* NEA-OECD Workshop Proceedings, 99-110.

Johnson, L.H., M. Niemeyer, G. Klubertanz, P. Siegel, and P. Gribi 2002. *Calculations of the temperature evolution of a repository for spent fuel, vitrified high-level waste and intermediate level waste in Opalinus Clay.* NAGRA (National Cooperative for the Disposal of Radioactive Waste), Technical Report 01-04.

Jung, J. et al. 2009. *Adagio 4.14 User's Guide*, SAND2009-7410, Sandia National Laboratories, Albuquerque, NM.

Knowles, M.K. and C.L. Howard, 1996. "Field and Laboratory Testing of Seal Materials Proposed for the Waste Isolation Pilot Plant." *Proceedings of the Waste Management 1996 Symposium, Tucson, AZ, February 25-29, 1996.* SAND95-2082C. Albuquerque, NM: Sandia National Laboratories.

Krumbein, W.C. and L.L. Sloss, 1963. *Stratigraphy and Sedimentation*. W.H. Freeman and Company, San Francisco, 660 p.

Krumhansl, J.L., 1983. "Near-surface heater test results: Environmental implications for the disposal of high-level waste." *Radioactive Waste Management and the Nuclear Fuel Cycle*, Volume 4(1). pp. 1-31.

Langmuir, D. 1997. Aqueous Environmental Chemistry, Prentice Hall, 600p.

Lappin, A.R., R.K. Thomas, and D. F. McVey 1981. *Eleana near-surface heater experiment final report*. SAND80-2137. Sandia National Laboratories, Albuquerque, NM.

Lee, J.O., W.J. Cho, et al. 1994. "Diffusion characteristics of iodide in a domestic bentonite of Korea." *Journal of the Korean Nuclear Society*. 26: 285-293.

Maes, A., C. Bruggeman, and J. Vancluysen 2004. "Reduction and Solubility Behaviour of Selenium under Boom Clay Conditions." *Proceedings : Euradwaste'04. Radioactive waste management community policy and research initiatives*. EUR-21027.

Martin, C.D., and G.W. Lanyon 2003. "Measurement of *in situ* stress in weak rocks at Mont Terri rock laboratory, Switzerland." *Int J Rock Mech Min Sci* 2003;40:1077–88.

McKinley, I.G. and A. Scholtis 1993. "A comparison of radionuclide sorption databases used in recent performance assessments." *Journal of Contaminant Hydrology* 13: 347-363.

Metz, V., B. Kienzler, and W. Schubler 2003. "Geochemical evaluation of different groundwater-host rock systems for radioactive waste disposal." *Journal of Contaminant Hydrology*, 61, 65-279.

NAGRA (National Cooperative for the Disposal of Radioactive Waste) 2002. *Project Opalinus Clay: Safety report demonstration of disposal feasibility for spent fuel, vitrified high-level waste and long-lived intermediate-level waste (Entsorgungsnachweis).* Technical Report 02-05.

National Academy of Sciences 1957. The disposal of radioactive waste on land. Publication 519.

Neuzil, C.E. 2000. "Osmotic generation of 'anomalous' fluid pressures in geologic environments." *Nature*, Vol. 403. pp. 182-184.

Notz, P.K., S.R. Subia, M.M. Hopkins, H. Moffat and D. Noble 2007. *Aria 1.5: User Manual*. SAND2007-2734, Sandia National Laboratories, Albuquerque, NM., 369p.

NEA (Nuclear Energy Agency) 2003. *Features, Events and Processes Evaluation Catalogue for Argillaceous Media.* Paris, France: Nuclear Energy Agency of the Organisation for Economic Co-Operation and Development.

NWTRB (Nuclear Waste Technical Review Board) 2009. Survey of National Programs for Managing High-Level Radioactive Waste and Spent Nuclear Fuel: A Report to Congress and the Secretary of Energy. http://www.nwtrb.gov/reports/nwtrb_survey_rpt.pdf

OECD NEA (Organization for Economic Co-operation and Development Nuclear Energy Agency) 1996. *Water, gas and solute movement through argillaceous media.* (prepared by S. T. Horseman, J.J.W. Higgo, J. Alexander, and J. F. Harrington) Report CC-96/1.

ORNL (Oak Ridge National Laboratory) 1986. *Proceedings of the first thermomechanical workshop for shale*. ORNL/Sub/85-97343/1.

Patrick, W.C. 1986. Spent fuel test—climax: An evaluation of the technical feasibility of geologic storage of spent nuclear fuel in granite. Lawrence Livermore National Laboratory. UCRL-53702.

Prashant, A. and D. Penumadu 2004. "Modeling the effect of overconsolidation on shear behavior of cohesive soils. In: Numerical Models in Geomechanics." NUMOG IX, Ottawa, Canada, 25-27 August 2004. G.N. Pande and S. Pietruszczak (eds.). Balkema Publishers, Taylor & Francis Group, London. pp. 131-138.

Ritter, D.F. 1967. "Rates of denudation." Journal Geol. Education, Vol. 15.

Sandia National Laboratories 2008a. *Postclosure Analysis of the Range of Design Thermal Loadings*. Sandia National Laboratories. ANL-NBS-HS-000057 Rev. 00. Las Vegas, Nevada: Sandia National Laboratories.

Sandia National Laboratories 2008b. *Features, Events, and Processes for the Total System Performance Assessment: Analyses.* ANL-WIS-MD-000027 REV 00. Las Vegas, Nevada: Sandia National Laboratories.

Sandia National Laboratories 2008c. *Total System Performance Assessment Model /Analysis for the License Application*. MDL-WIS-PA-000005 REV 00 AD 01. Las Vegas, Nevada: Sandia National Laboratories.

Schwartz, F., and H. Zhang 2003, *Fundamentals of Groundwater*, Chapter 23. Modeling Contaminant Transport, John Wiley and Sons, 592 p.

Schwyn, B. and P. Wersin 2004. "The compilation of geochemical data bases for performance assessment of a planned repository in the Opalinus clay in Northern Switzerland." Material Research Society Symposium Proceedings, 807, 1-6.

Shurr, G.W. 1977. *The Pierre Shale, Northern Great Plains; A Potential Isolation Medium for Radioactive Waste.* United States Geological Survey Open File Report 77-776.

Sobolik, S.R., M. Itamura, C.M. Stone, S.W. Webb 2002. "Predictions of Bentonite Behavior for Thermo-Hydro-Mechanical Simulation of FEBEX Drift: Task 1, Part B." DOE Report to UPC, Sandia National Laboratories, Albuquerque, NM.

Swift, P., G. Barr, R. Barnard, R.P. Rechard, A. Schenker, G. Freeze, and P. Burck 1999. "Feature, Event, and Process Screening and Scenario Development for the Yucca Mountain Total System Performance Assessment." *Proceedings of the NEA Workshop on Scenario Development, Madrid, Spain, May 10-12, 1999, Paris, France: Nuclear Energy Agency of the* Organisation for Economic Co-operation and Development.

Uhlig L., M. Jobmann, M. Polster, J. Vaunat, B. Garrite, and Y. Wileveau 2007. "Stress redistribution and hydromechanical effects due to excavation and drilling operations in TER experiment." In: Proceedings, International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement, Lille, France, September 17-18, 2007.

van Genuchten, M.T. 1980. "A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils." *Soil Science Society of America Journal*, 44, (5), 892-898. Madison, Wisconsin: Soil Science Society of America.

Volckaert G., L. Ortiz, P. de Canière, M. Put, S.T. Horseman, J.F. Harrington, V. Fioravante, and M. Impey 1995. MEGAS: *Modelling and Experiments on Gas Migration in Repository Host Rock*. 447 pp. EUR-16235, Luxemburg, E.C.

Volckaert, F., X. Bernier, X. Sillen, M. Van Geet, J.-C. Mayor, I. Göbel, P. Blümling, B. Frieg, and K. Su 2005. "Similarities and Differences in the Behaviour of Plastic and Indurated Clays." In: *Proceedings, Euradwaste'04. Radioactive waste management community policy and research initiatives*. EUR-21027, pp. 281-291.

Wersin, P. 2003. "Geochemical modeling of bentonite porewater in high-level waste repositories." *Journal of Contaminant Hydrology*, 61, 405-422.

Wileveau, Y. and K. Su 2007. "*In situ* thermal experiments carried out in Opalinus clay and Callovo-Oxfordian claystones by ANDRA – Experiment set-up and measurement results." In: *Proceedings, International Meeting on Clays in Natural and Engineered Barriers for Radioactive Waste Confinement.* Lille, France. September 17-18, 2007.

Zhang, C.L. and T. Rothfuchs 2007. *Laboratory experiments on the THM behaviour of clay rocks*. Final Repository Safety Research Division, Braunschweig – Germany (GRS). European Commission, Euratom Research and Training Programme on Nuclear Energy, TIMODAZ Project Report WP-2.

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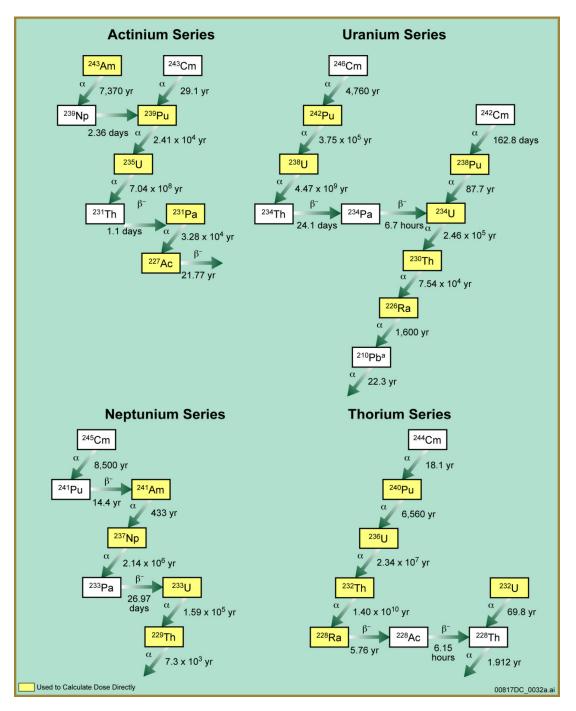
APPENDIX A: U.S. HLW AND UNF INVENTORY

In 2007, DOE estimated that 109,300 metric tons heavy metal (MTHM) of high-level waste and spent nuclear fuel in the U.S. will ultimately need to be stored (DOE Office of Public Affairs, August 5, 2008). This inventory consists of 70,000 MTHM that is included in the Yucca Mountain license application, with the remainder that will need to be disposed of from future activities. The inventory includes CSNF, DSNF, and HLWG. The inventory consists of actinide elements in several radionuclide decay chains (Figure A-1) along with a number of fission products.

The 70,000 MTHM Yucca Mountain inventory is predominantly (about 90%) CSNF, which in turn consists of spent fuel assemblies from PWRs and BWRs. A representative inventory, showing the important actinide elements from Figure A-1 and the important fission products, for a single Yucca Mountain waste package is provided in Table A-1 (Brady et al. 2009). The 31-radionuclide inventory is shown for an initial time (either 2030 or 2067 depending on waste type) and aged to a common year, 2117, about 100 years from the present. Note that this table actually represents two different types of waste packages: a CSNF waste package that contains the CSNF inventory (a single CSNF waste package would contain either 21 PWR assemblies or 44 BWR assemblies); and a codisposal waste package that combines the DSNF and HLWG inventory. Also, note that the inventories in Table A-1 do not include any mixed oxide fuel or lanthanide borosilicate glass waste.

For the purposes of discussing and characterizing the waste for clay disposal, the relative radionuclide inventories for CSNF shown in Table A-1 are considered representative of the entire U.S. HLW and UNF inventory (Brady et al. 2009). The other waste streams (DSNF and HLWG) contain similar relative radionuclide inventories (Table A-1) as the CSNF waste stream.

By weight, CSNF is about 97% ²³⁸U, with contributions of 0.3% to 0.8% from ²³⁵U, ²³⁶U, ²³⁹Pu, and ²⁴⁰Pu. All other radionuclides contribute less than 0.1%. Figure A-2 shows the relative contributions of the 31 radionuclides by activity (in Curies), which is a more direct indicator of their potential effect on dose (Brady et al. 2009). Note that Figure A-2 includes all waste (not just CSNF), but the relative contributions apply reasonably well to all waste streams. The change in importance of the various radionuclides over time is indicative of the effects of decay and ingrowth. The same information is tabulated in Table A-2, which also shows the decline in total activity over time.



Source: SNL 2008c, Figure 6.3.7-4.

^a A series of short-lived daughters between ²²⁶Ra and ²¹⁰Pb are not shown. Also, ²¹⁰Pb is not used to calculate dose directly, but its biosphere dose conversion factor is included with that of ²²⁶Ra.

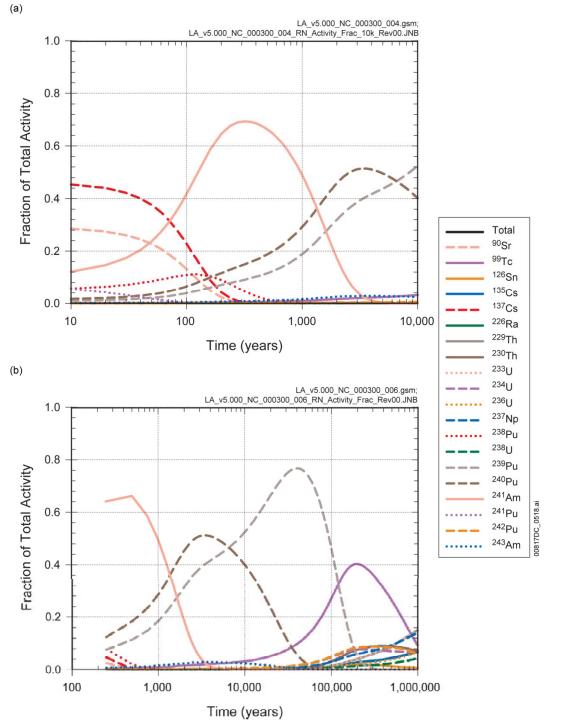
^b Value listed under each radionuclide is the approximate decay half-life for the radionuclide.

Figure A-1. Decay Chains of the Actinide Elements

	Waste Package Inventory (g/pkg)					
Radionuclide	CSNF at 2067	CSNF after 50 Years	DSNF at 2030	DSNF after 87 Years	HLWG at 2030	HLWG after 87 Years
²²⁷ Ac	2.47E-06	6.27E-06	1.22E-03	1.39E-03	1.91E-04	9.47E-04
²⁴¹ Am	8.18E+03	9.84E+03	2.18E+02	2.15E+02	3.75E+01	3.37E+01
²⁴³ Am	1.24E+03	1.23E+03	6.73E+00	6.68E+00	5.75E-01	5.70E-01
¹⁴ C	1.35E+00	1.34E+00	1.81E+00	1.79E+00	0.00E+00	0.00E+00
³⁶ CI	3.23E+00	3.23E+00	4.23E+00	4.23E+00	0.00E+00	0.00E+00
²⁴⁵ Cm	1.75E+01	1.74E+01	9.25E-02	9.18E-02	5.43E-02	5.39E-02
¹³⁵ Cs	4.36E+03	4.36E+03	9.74E+01	9.74E+01	1.27E+02	1.27E+02
¹³⁷ Cs	5.90E+03	1.86E+03	9.72E+01	1.31E+01	3.02E+02	4.07E+01
¹²⁹	1.73E+03	1.73E+03	3.56E+01	3.56E+01	7.27E+01	7.27E+01
²³⁷ Np	4.57E+03	5.32E+03	8.14E+01	1.12E+02	9.95E+01	1.04E+02
²³¹ Pa	9.17E-03	1.22E-02	2.14E+00	2.14E+00	1.53E+00	1.53E+00
²³⁸ Pu	1.52E+03	1.02E+03	1.25E+01	6.28E+00	3.91E+01	1.96E+01
²³⁹ Pu	4.32E+04	4.31E+04	2.21E+03	2.20E+03	5.58E+02	5.57E+02
²⁴⁰ Pu	2.05E+04	2.04E+04	4.35E+02	4.31E+02	4.61E+01	4.57E+01
²⁴¹ Pu	2.66E+03	2.40E+02	2.92E+01	4.49E-01	1.22E+00	1.89E-02
²⁴² Pu	5.28E+03	5.28E+03	3.02E+01	3.02E+01	3.89E+00	3.89E+00
²²⁶ Ra	0.00E+00	1.29E-04	4.57E-05	1.80E-04	2.42E-05	2.68E-05
²²⁸ Ra	0.00E+00	1.90E-11	1.51E-05	8.77E-06	6.00E-06	1.20E-05
⁷⁹ Se	4.19E+01	4.19E+01	6.82E+00	6.82E+00	7.01E+00	7.01E+00
¹²⁶ Sn	4.63E+02	4.63E+02	9.40E+00	9.40E+00	1.70E+01	1.70E+01
⁹⁰ Sr	2.49E+03	7.46E+02	5.22E+01	6.43E+00	1.74E+02	2.14E+01
⁹⁹ Tc	7.55E+03	7.55E+03	1.58E+02	1.58E+02	1.01E+03	1.01E+03
²²⁹ Th	0.00E+00	2.07E-05	3.24E-01	5.22E-01	3.30E-03	1.05E-02
²³⁰ Th	1.52E-01	4.32E-01	1.18E-01	2.33E-01	8.12E-04	9.02E-03
²³² Th	0.00E+00	5.63E-02	2.17E+04	2.17E+04	2.98E+04	2.98E+04
²³² U	1.02E-02	6.20E-03	1.28E+00	5.39E-01	4.08E-04	1.72E-04
²³³ U	5.76E-02	1.37E-01	5.38E+02	5.38E+02	1.94E+01	1.94E+01
²³⁴ U	1.75E+03	2.24E+03	4.73E+02	4.79E+02	2.33E+01	4.24E+01
²³⁵ U	6.26E+04	6.27E+04	2.51E+04	2.51E+04	1.41E+03	1.41E+03
²³⁶ U	3.84E+04	3.85E+04	1.25E+03	1.25E+03	5.99E+01	6.03E+01
²³⁸ U	7.82E+06	7.82E+06	6.84E+05	6.84E+05	2.37E+05	2.37E+05

Table A-1. Yucca Mountain Nuclear Waste Inventory per Waste Package by Radionuclide

Source: SNL 2008c, Table 6.3.7-4a.



Source: SNL 2008c, Figure 8.3-2.

Figure A-2. Mean Radionuclide Contributions to the Total Yucca Mountain Nuclear Waste Inventory as a Function of Time for (a) 10,000 Years and (b) 1,000,000 Years after 2117

Time After Closure, 2117 (yr)	Percent of Total Initial Curie Inventory	Major Contributors to Total Inventory at Time after Closure
0	100.00	¹³⁷ Cs (46%), ⁹⁰ Sr (29%), ²⁴¹ Am (10%)
10	81.2	¹³⁷ Cs (45%), ⁹⁰ Sr (28%), ²⁴¹ Am (12%)
100	20.75	²⁴¹ Am (41%), ¹³⁷ Cs (22%), ⁹⁰ Sr (13%), ²³⁸ Pu (11%))
1,000	4.20	²⁴¹ Am (48%), ²⁴⁰ Pu (29%), ²³⁹ Pu (19%)
10,000	1.18	²³⁹ Pu (52%), ²⁴⁰ Pu (40%)
100,000	0.10	²³⁹ Pu (46%), ⁹⁹ Tc (27%)
500,000	0.03	⁹⁹ Tc (26%), ²²⁹ Th (9%), ²³⁰ Th (9%), ²²⁶ Ra (9%), ²³³ U (9%), ²³⁷ Np (9%), ²⁴² Pu (8%), ²³⁴ U (7%)
1,000,000	0.02	 ²³³U (15%), ²²⁹Th (15%), ²³⁷Np (14%), ⁹⁹Tc (9%), ²³⁰Th (7%), ²²⁶Ra (7%), ¹³⁵Cs (7%), ²³⁶U (6%), ²⁴²Pu (6%)

Table A-2.Decay of Total Yucca Mountain Nuclear Waste Inventory as a Function of Time, and
Dominant Contributors to Total Curie Inventory

Source: SNL 2008c, Table 8.3-1.

At early time (the first few hundred years after emplacement), the radionuclides with the highest activity are all short-lived (half-lives less than 500 years): ¹³⁷Cs, ⁹⁰Sr, ²⁴¹Am, and ²³⁸Pu. From about 100 years to 1,500 years after emplacement, ²⁴¹Am is the largest contributor to the total activity. Subsequent to that, moderate half-life radionuclides become more important. ²⁴⁰Pu (half-life of 6,560 years) is the largest contributor to total activity from about 1,500 years to 7,000 years after emplacement, then ²³⁹Pu (half-life of 24,100 years) becomes the largest contributor until about 100,000 yr after emplacement. At very long times (greater than 100,000 years after emplacement), the following long-lived radionuclides become most important to total activity: ⁹⁹Tc, ²⁴²Pu, ²³⁷Np, ²³⁴U, ²³⁰Th, ²²⁶Ra, ²³³U, ²²⁹Th, ¹³⁵Cs, and ²³⁶U.

Table A-2 shows that the total activity (in Curies) of the inventory decays to about 20% of the initial activity after 100 years, to about 4% after 1,000 years, and to about 1% of the initial activity after 10,000 years. Roughly 1,000 years is required before the total radioactivity in UNF would decay to the background level of a 0.2% U ore body. The radiation in un-processed spent fuel requires roughly 10,000 years to decay to the background levels of an ore body (Langmuir 1997).

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APPENDIX B: SCREENING DECISIONS OF GENERIC FEPS FOR REPOSITORY IN CLAY/SHALE

Table B-1 summarizes the screening decisions for 216 FEPs (i.e., whether a FEP is likely to need to be included in or excluded from a full performance assessment for a clay/shale repository). Table B-1 also includes a qualitative estimate of the level of effort likely to be required to provide a basis for the screening decision. For excluded FEPs, "1" means the technical or regulatory basis is readily available and all that is needed is documentation, "2" means new technical work likely is needed, and "3" indicates a potentially significant amount of work is needed. For included FEPs, "1" indicates that this is a normal part of modeling, "2" indicates that this is a significant aspect of the modeling, and "3" indicates possible modeling challenges. Notes entered in this column provide clarification about how the FEP may need to be considered for clay/shale disposal.

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
0.0.00.00	0. ASSESSMENT BASIS						
0.1.02.01	Timescales of Concern			Include	1		0.1.02.00.0A
0.1.03.01	Spatial Domain of Concern	Size and geometry of host rock, surrounding units of geosphere, and biosphere		Include	1	A1.1.1	0.1.03.00.0A
0.1.09.01	Regulatory Requirements and Exclusions			Include	3 Regulations will need to be revised		0.1.09.00.0A
0.1.10.01	Model Issues	 Conceptual model Mathematical implementation Geometry and dimensionality Process coupling Boundary and initial conditions 		Include	1		0.1.10.00.0A
0.1.10.02	Data Issues	 Parameterization and values Correlations Uncertainty 		Include	1		0.1.10.00.0A
1.0.00.00	1. EXTERNAL FACTORS						
1.1.00.00	1. REPOSITORY ISSUES						
1.1.01.01	Open Boreholes	 Site investigation boreholes (open, improperly sealed) Preclosure and postclosure monitoring boreholes Enhanced flow pathways from EBS 		Exclude	1		1.1.01.01.0A 1.1.11.00.0A
1.1.02.01	Chemical Effects from Preclosure Operations - In EBS - In EDZ - In Host Rock	 Water contaminants (explosives residue, diesel, organics, etc.) Water chemistry different than host rock (e.g., oxiding) Undesirable materials left Accidents and unplanned events 		Exclude	1		1.1.02.00.0A 1.1.02.03.0A 1.1.12.01.0A 2.2.01.01.0B

Table B-1. Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
1.1.02.02	Mechanical Effects from Preclosure Operations - In EBS - In EDZ - In Host Rock	 Creation of excavation-disturbed zone (EDZ) Stress relief Boring and blasting effects Rock reinforcement effects (drillholes) Accidents and unplanned events Enhanced flow pathways [see also Evolution of EDZ in 2.2.01.01] 		Exclude	1		1.1.01.01.0B 1.1.02.00.0B 1.1.12.01.0A 2.2.01.01.0A
1.1.02.03	Thermal-Hydrologic Effects from Preclosure Operations - In EBS - In EDZ - In Host Rock	 Site flooding Preclosure ventilation Accidents and unplanned events 		Exclude	1		1.1.02.01.0A 1.1.02.02.0A 1.1.12.01.0A
1.1.08.01	Deviations from Design and Inadequate Quality Control	 Error in waste emplacement (waste forms, waste packages, waste package support materials) Error in EBS component emplacement (backfill, seals, liner) Inadequate excavation / construction (planning, schedule, implementation) Aborted / incomplete closure of repository Material and/or component defects 		Exclude	1		1.1.03.01.0A 1.1.03.01.0B 1.1.04.01.0A 1.1.07.00.0A 1.1.08.00.0A 1.1.09.00.0A
1.1.10.01	Control of Repository Site	 Active controls (controlled area) Retention of records Passive controls (markers) 		Exclude	1		1.1.05.00.0A 1.1.10.00.0A
1.1.13.01	Retrievability			Include	1 However, the U.S. may reconsider current policy		1.1.13.00.0A

Table B-1. Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria (continued)

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
1.2.00.00	2. GEOLOGICAL PROCESSES AND EFFECTS						
1.2.01.00	2.01. LONG-TERM PROCESSES						
1.2.01.01	Tectonic Activity – Large Scale	- Uplift - Folding		Exclude	1	C2.1	1.2.01.01.0A
1.2.02.01	Subsidence			Exclude	1		2.2.06.04.0A
1.2.05.01	Metamorphism	 Structural changes due to natural heating and/or pressure 		Exclude	1		1.2.05.00.0A
1.2.08.01	Diagenesis	 Mineral alteration due to natural processes 		Exclude	1		1.2.08.00.0A
1.2.09.01	Diapirism	 Plastic flow of rocks under lithostatic loading Salt / evaporates Clay 		Include	3 Modeling capability exists but U.S. tests required for constitutive equations		1.2.09.00.0A 1.2.09.01.0A
1.2.10.01	Large-Scale Dissolution			Exclude	1		1.2.09.02.0A
1.2.03.00	2.03.SEISMIC ACTIVITY						
1.2.03.01	Seismic activity impacts EBS and/or EBS components	 Mechanical damage to EBS (from ground motion, rockfall, drift collapse, fault displacement) [see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, 2.1.07.08, and 2.1.07.10] 	SYS - DE	Exclude	1		1.2.02.03.0A 1.2.03.02.0A 1.2.03.02.0B 1.2.03.02.0C
1.2.03.02	Seismic activity impacts geosphere	- Future faults alter flow pathways and change hydraulic parameters	SYS-DE	Exclude	1	C2.2	

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
1.2.04.00	2.04. IGNEOUS ACTIVITY						
1.2.04.01	Igneous activity impacts EBS and/or EBS components	 Mechanical damage to EBS (from igneous intrusion) Chemical interaction with magmatic volatiles Transport of radionuclides (in magma, pyroclasts, vents) [see also Mechanical Impacts in 2.1.07.04, 2.1.07.05, 2.1.07.06, 2.1.07.07, and 2.1.07.08] 	SYS- DE	Exclude	1		1.2.04.03.0A 1.2.04.04.0A 1.2.04.04.0B 1.2.04.05.0A 1.2.04.06.0A
1.2.04.01	Geothermal regime	- Present and future geothermal regime	SYS-DE	Exclude	1	C1.2.1	
1.3.00.00	3. CLIMATIC PROCESSES AND EFFECTS						
1.3.01.01	Climate Change - Natural	 Variations in precipitation and temperature Long-term global Short-term regional and local [see also Human Influences on Climate in 1.4.01.01] [contributes to Precipitation in 2.3.08.01, Surface Runoff and Evapotranspiration in 2.3.08.02] 		Include	1		1.3.01.00.0A
1.3.04.01	Periglacial Effects	- Permafrost - Seasonal freeze/thaw		Exclude?	1 Decision would depend upon location in U.S.		1.3.04.00.0A
1.3.05.01	Glacial and Ice Sheet Effects	 Glaciation Isostatic depression Future stress regime Melt water 		Exclude?	1 Decision would depend upon location in U.S.	C2.6	1.3.05.00.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
1.4.00.00	4. FUTURE HUMAN ACTIONS						
1.4.01.01	Human Influences on Climate - Intentional	 Variations in precipitation and temperature Global, regional, and/or local Greenhouse gases, ozone layer failure [see also Climate Change in 1.3.01.01] 		Exclude	1		1.4.01.00.0A 1.4.01.01.0A 1.4.01.02.0A 1.4.01.04.0A
1.4.02.01	Human Influences on Climate - Accidental	 Variations in precipitation and temperature Global, regional, and/or local Greenhouse gases, ozone layer failure [see also Climate Change in 1.3.01.01] 		Exclude	2 Judge allowed Nevada contention on this topic for hearings		1.4.01.00.0A 1.4.01.01.0A 1.4.01.02.0A 1.4.01.04.0A
1.4.03.01	Human Intrusion - Deliberate	 Drilling (resource exploration,) Mining / tunneling Unintrusive site investigation (airborne, surface-based,) [see also Control of Repository Site in 1.1.10.01] 	SYS – DE	Exclude	1		1.4.02.01.0A 1.4.02.02.0A 1.4.03.00.0A 1.4.04.00.0A 1.4.04.01.0A 1.4.05.00.0A 3.3.06.01.0A
1.4.04.01	Human Intrusion - Inadvertent	 Drilling (resource exploration,) Mining / tunneling Unintrusive site investigation (airborne, surface-based,) [see also Control of Repository Site in 1.1.10.01] 	SYS – DE	Include	1 Need regulatory clarification; 40 CFR 191 and 40 CFR 197 both include but differ in how modeled and whether to include in hazard measure		1.4.02.01.0A 1.4.02.02.0A 1.4.03.00.0A 1.4.04.00.0A 1.4.04.01.0A 1.4.05.00.0A 3.3.06.01.0A

Table B-1. Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria (continued)

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
1.4.11.01	Explosions and Crashes from Human Activities	 War Sabotage Testing Resource exploration / exploitation Aircraft 		Exclude	1		1.4.11.00.0A
1.5.00.00	5. OTHER						
1.5.01.01	Meteorite Impact	 Cratering, host rock removal Exhumation of waste Alteration of flow pathways 		Exclude	1		1.5.01.01.0A
1.5.01.02	Extraterrestrial Events	 Solar systems (supernova) Celestial activity (sun - solar flares, gamma-ray bursters; moon – earth tides) Alien life forms 		Exclude	1		1.5.01.02.0A 1.5.03.02.0A
1.5.03.01	Earth Planetary Changes	 Changes in earth's magnetic field Changes in earth's gravitational field (tides) 		Exclude	1		1.5.03.01.0A 1.5.03.02.0A
2.0.00.00	2. DISPOSAL SYSTEM FACTORS						
2.1.00.00	1. WASTES AND ENGINEERED FEATURES						
2.1.01.00	1.01. INVENTORY						
2.1.01.01	Waste Inventory - Radionuclides - Non-Radionuclides	- Composition - Enrichment / Burn-up	WF	Include	1		2.1.01.01.0A
2.1.01.02	Radioactive Decay and Ingrowth		EBS (TRAN)	Include	1		3.1.01.01.0A
2.1.01.03	Heterogeneity of Waste Inventory - Waste Package Scale - Repository Scale	- Composition - Enrichment / Burn-up - Damaged Area	WF-WP	Include	1		2.1.01.03.0A 2.1.01.04.0A
2.1.01.04	Interactions Between Co- Located Waste		WF-WP	Include	1		2.1.01.02.0A 2.1.01.02.0B

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.02.00	1.02. WASTE FORM						
2.1.02.01	CSNF (Commercial SNF) Degradation - Alteration / Phase Separation - Dissolution / Leaching - Radionuclide Release	Degradation is dependent on: - Composition - Geometry / Structure - Enrichment / Burn-up - Surface Area - Gap and Grain Fraction - Damaged Area - THC Conditions [see also Mechanical Impact in 2.1.07.06 and Thermal-Mechanical Effects in 2.1.11.06]	WF	Include	1		2.1.02.02.0A 2.1.02.01.0A 2.1.02.28.0A 2.1.02.07.0A
2.1.02.06	CSNF Cladding Degradation and Failure	 Initial damage General Corrosion Microbially Influenced Corrosion Localized Corrosion (silica, fluoride) Enhanced Corrosion (silica, fluoride) Stress Corrosion Cracking Hydride Cracking Unzipping Creep Internal Pressure Mechanical Impact 	WF	Include	2 If modeled as initially failed, then inclusion simple: yet, if common mode failure with package failure can be diminished then inclusion provides an additional barrier but must select mode of cladding degradation for modeling		2.1.02.11.0A 2.1.02.12.0A 2.1.02.13.0A 2.1.02.13.0A 2.1.02.15.0A 2.1.02.15.0A 2.1.02.15.0A 2.1.02.17.0A 2.1.02.17.0A 2.1.02.27.0A 2.1.02.27.0A 2.1.02.22.0A 2.1.02.23.0A 2.1.02.25.0B 2.1.02.25.0B 2.1.02.25.0B 2.1.02.25.0B 2.1.02.26.0A 2.1.02.20.0A 2.1.02.20.0A 2.1.02.24.0A 2.1.09.03.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.02.01	DSNF (DOE-owned SNF) Degradation - Alteration / Phase Separation - Dissolution / Leaching - Radionuclide Release	Degradation is dependent on: - Composition - Geometry / Structure - Enrichment / Burn-up - Surface Area - Gap and Grain Fraction - Damaged Area - THC Conditions [see also Mechanical Impact in 2.1.07.06 and Thermal-Mechanical Effects in 2.1.11.06]	WF	Exclude	1		2.1.02.02.0A 2.1.02.01.0A 2.1.02.28.0A 2.1.02.07.0A
2.1.02.06	DSNF Cladding Degradation and Failure	 Initial damage General Corrosion Microbially Influenced Corrosion Localized Corrosion (silica, fluoride) Stress Corrosion Cracking Hydride Cracking Unzipping Creep Internal Pressure Mechanical Impact 	WF	Exclude	1		2.1.02.11.0A 2.1.02.12.0A 2.1.02.13.0A 2.1.02.14.0A 2.1.02.15.0A 2.1.02.17.0A 2.1.02.17.0A 2.1.02.27.0A 2.1.02.27.0A 2.1.02.21.0A 2.1.02.23.0A 2.1.02.25.0A 2.1.02.25.0B 2.1.02.25.0B 2.1.02.26.0A 2.1.02.20.0A 2.1.02.20.0A 2.1.02.24.0A 2.1.09.03.0A

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UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

Number	Phenomena	Associated Processes	Domain	Screening Decision	Level of Effort	FEP	Database
2.1.02.01	NSNF (Naval SNF) Degradation - Alteration / Phase Separation - Dissolution / Leaching - Radionuclide Release	Degradation is dependent on: - Composition - Geometry / Structure - Enrichment / Burn-up - Surface Area - Gap and Grain Fraction - Damaged Area - THC Conditions [see also Mechanical Impact in 2.1.07.06 and Thermal-Mechanical Effects in 2.1.11.06]	WF	Include	1 Model with CSNF as a surrogate		2.1.02.02.0A 2.1.02.01.0A 2.1.02.28.0A 2.1.02.07.0A
2.1.02.06	NSNF Cladding Degradation and Failure	 Initial damage General Corrosion Microbially Influenced Corrosion Localized Corrosion (silica, fluoride) Stress Corrosion Cracking Hydride Cracking Unzipping Creep Internal Pressure Mechanical Impact 	WF	Exclude	1 Model with as CSNF as a surrogate		2.1.02.11.0A 2.1.02.12.0A 2.1.02.13.0A 2.1.02.14.0A 2.1.02.15.0A 2.1.02.15.0A 2.1.02.17.0A 2.1.02.17.0A 2.1.02.27.0A 2.1.02.27.0A 2.1.02.22.0A 2.1.02.23.0A 2.1.02.25.0B 2.1.02.25.0B 2.1.02.25.0B 2.1.02.25.0B 2.1.02.25.0B 2.1.02.26.0A 2.1.02.20.0A 2.1.02.20.0A 2.1.02.20.0A 2.1.02.24.0A 2.1.02.24.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.02.02	HLW (Glass, Ceramic, Metal) Degradation - Alteration / Phase Separation - Dissolution / Leaching - Cracking - Radionuclide Release	Degradation is dependent on: - Composition - Geometry / Structure - Surface Area - Damaged / Cracked Area - Mechanical Impact - THC Conditions [see also Mechanical Impact in 2.1.07.07 and Thermal-Mechanical Effects in 2.1.11.06]	WF	Include	1		2.1.02.03.0A 2.1.02.05.0A
2.1.02.04	HLW (Glass, Ceramic, Metal) Recrystallization		WF	Exclude	1		2.1.02.06.0A
2.1.02.03	Degradation of Organic/Cellulosic Materials in Waste	[see also Complexation in EBS in 2.1.09.54]	WF	Exclude	1		2.1.02.10.0A
2.1.02.05	Pyrophoricity or Flammable Gas from SNF or HLW	[see also Gas Explosions in EBS in 2.1.12.04]	WF	Exclude	1		2.1.02.08.0A 2.1.02.29.0A
2.1.03.00	1.03. WASTE CONTAINER						
2.1.03.01	Early Failure of Waste Packages	 Manufacturing defects Improper sealing [see also Deviations from Design in 1.1.08.01] 	WP	Exclude?	1 Importance of early failure dependent upon whether corrosion resistant package used		2.1.03.08.0A
2.1.03.02	General Corrosion of Waste Packages	 Dry-air oxidation Humid-air corrosion Aqueous phase corrosion Passive film formation and stability 	WP	Exclude?	1 Importance of corrosion dependent upon whether corrosion resistant package used		2.1.03.01.0A
2.1.03.03	Stress Corrosion Cracking (SCC) of Waste Packages	 Crack initiation, growth and propagation Stress distribution around cracks 	WP	Exclude?	1		2.1.03.02.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.03.04	Localized Corrosion of Waste Packages	- Pitting - Crevice corrosion - Salt deliquescence [see also 2.1.09.06 Chemical Interaction with Backfill]	WP	Exclude?	1		2.1.03.03.0A 2.1.09.28.0A
2.1.03.05	Hydride Cracking of Waste Packages	 Hydrogen diffusion through metal matrix Crack initiation and growth in metal hydride phases 	WP	Exclude?	1		2.1.03.04.0A
2.1.03.06	Microbially Influenced Corrosion (MIC) of Waste Packages		WP	Exclude?	1		2.1.03.05.0A
2.1.03.07	Internal Corrosion of Waste Packages Prior to Breach		WP	Exclude	1		2.1.03.06.0A
2.1.03.08	Evolution of Flow Pathways in Waste Packages	 Evolution of physical form of waste package Plugging of cracks in waste packages [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impacts in 2.1.07.05, 2.1.07.06, and 2.1.07.07, Thermal-Mechanical Effects in 2.1.11.06 and 2.1.11.07] 	WP	Exclude?	1		2.1.03.10.0A 2.1.03.11.0A
2.1.04.00	1.04. BUFFER / BACKFILL						
2.1.04.01	Evolution of Backfill	 Alteration Thermal expansion / Degradation Swelling / Compaction Erosion / Dissolution Evolution of backfill flow pathways [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Mechanical Impact in 2.1.07.04, Thermal-Mechanical Effects in 2.1.11.08, Chemical Interaction in 2.1.09.06] 	BUFF	Include	1	B3.3 B4.1 B5.2 B5.3 C2.3 C2.4	2.1.04.05.0A 2.1.04.03.0A

Table B-1. Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria (continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.05.00	1.05. SEALS						
2.1.05.01	Evolution of Seals	 Alteration / Degradation / Cracking Erosion / Dissolution [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 	SL	Include	1		2.1.05.03.0A
		2.1.09.08]					
2.1.06.00	1.06. OTHER EBS MATERIALS						
2.1.06.01	Degradation of Liner / Rock Reinforcement Materials in EBS	 Alteration / Degradation / Cracking Corrosion Erosion / Dissolution / Spalling [see also Mechanical Impact in 2.1.07.08, Thermal-Mechanical Effects in 2.1.11.09, Chemical Interaction in 2.1.09.07] 	SL	Exclude?	1 Placement would depend on clay/shale stability		2.1.06.02.0A
2.1.07.00	1.07. MECHANICAL PROCESSES						
2.1.07.01	Rockfall	- Dynamic loading (block size and velocity) [see also Mechanical Effects on Host Rock in 2.2.07.01]	EBS-NF	Exclude	1		2.1.07.01.0A
2.1.07.02	Drift Collapse	 Static loading (rubble volume) Alteration of seepage Alteration of EBS flow pathways Alteration of EBS thermal environment [see also Evolution of Flow Pathways in EBS in 2.1.08.06, Chemical Effects of Drift Collapse in 2.1.09.12, and Effects of Drift Collapse on TH in 2.1.11.04, Mechanical Effects on Host Rock in 2.2.07.01] 	EBS-NF	Include	2 Closure and healing of EDZ important aspect of clay/shale repository to demonstrate understanding but has little influence on long-term performance		2.1.07.02.0A 1.2.03.02.0D

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.07.03	Mechanical Effects of Backfill	 Protection of other EBS components from rockfall / drift collapse 	BUFF	Include	2		2.1.04.04.0A
2.1.07.04	Mechanical Impact on Backfill	 Rockfall / Drift collapse Hydrostatic pressure Internal gas pressure [see also Degradation of Backfill in 2.1.04.01 and Thermal-Mechanical Effects in 2.1.11.08] 	BUFF-NF	Include	2		2.1.04.05.0A
2.1.07.05	Mechanical Impact on Waste Packages	 Rockfall / Drift collapse Waste package movement Hydrostatic pressure Internal gas pressure Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.07] 	WP- BUFF	Include	2		2.1.03.07.0A 2.1.07.04.0A 2.1.09.03.0B
2.1.07.06	Mechanical Impact on SNF Waste Form	- Drift collapse - Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.06]	WF-WP	Include	2		2.1.07.02.0A 2.1.09.03.0B
2.1.07.07	Mechanical Impact on HLW Waste Form	- Drift collapse - Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.06]	WF-WP	Include	2		2.1.07.02.0A 2.1.09.03.0B
2.1.07.08	Mechanical Impact on Other EBS Components - Seals - Liner/Rock Reinforcement Materials - Waste Package Support Materials	 Rockfall / Drift collapse Movement Hydrostatic pressure Swelling corrosion products [see also Thermal-Mechanical Effects in 2.1.11.09] 	SL-NF	Include	2		2.1.07.02.0A 2.1.09.03.0C
2.1.07.09	Mechanical Effects at EBS Component Interfaces	 Component-to-component contact (static or dynamic) 	EBS (MECH)	Include	2		2.1.06.07.0B 2.1.08.15.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.07.10	Mechanical Degradation of EBS	 Floor buckling Fault displacement Initial damage from excavation / construction Consolidation of EBS components Degradation of waste package support structure Alteration of EBS flow pathways [see also Mechanical Effects from Preclosure in 1.1.02.02, Evolution of Flow Pathways in EBS in 2.1.08.06, Drift Collapse in 2.1.07.02, Degradation in 2.1.04.01, 2.1.05.01, and 2.1.06.01, and Mechanical Effects on Host Rock in 2.2.07.01] 	EBS (MECH)	Include	2		2.1.06.05.0B 2.1.07.06.0A 1.2.02.03.0A 2.1.08.15.0A
2.1.08.00	1.08. HYDROLOGIC PROCESSES						
2.1.08.01	Flow Through the EBS	 Saturated / Unsaturated flow Preferential flow pathways Density effects on flow Initial hydrologic conditions Flow pathways out of EBS Hydraulic properties [see also Open Boreholes in 1.1.01.01, Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Flow in Waste Packages in 2.1.08.02, Flow in Backfill in 2.1.08.03, Flow through Seals 2.1.08.04, Flow through Liner in 2.1.08.05, Thermal Effects on Flow in 2.1.11.10, Effects of Gas on Flow in 2.1.12.02]	EBS (FLOW)	Include	1		2.1.08.09.0A 2.1.08.07.0A 2.1.08.05.0A
2.1.08.02	Flow In and Through Waste Packages	 Saturated / Unsaturated flow Movement as thin films or droplets 	WP	Include	1		2.1.03.10.0A 2.1.03.11.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.08.03	Flow in Backfill	- Fracture / Matrix flow	BUFF	Include	1	B5.2 B5.3 C2.3 C2.4	2.1.04.01.0A
2.1.08.04	Flow Through Seals		SL	Include	1		2.1.05.01.0A
2.1.08.05	Flow Through Liner / Rock Reinforcement Materials in EBS		SL	Include	1		2.1.06.04.0A
2.1.08.06	Alteration and Evolution of EBS Flow Pathways	 Drift collapse Degradation/consolidation of EBS components Plugging of flow pathways Formation of corrosion products Water ponding [see also Evolution of Flow Pathways in WPs in 2.1.03.08, Evolution of Backfill in 2.1.04.01, Drift Collapse in 2.1.07.02, and Mechanical Degradation of EBS in 2.1.07.10] 	EBS (FLOW)	Include	1		2.1.08.12.0A 2.1.08.15.0A 2.1.03.10.0A 2.1.03.11.0A 2.1.09.02.0A
2.1.08.07	Condensation Forms in Repository - On Drift Roof / Walls - On EBS Components	 Heat transfer (spatial and temporal distribution of temperature and relative humidity) Dripping [see also Heat Generation in EBS in 2.1.11.01, Effects on EBS Thermal Environment in 2.1.11.03 and 2.1.11.04] 	EBS (T- H)	Exclude	1		2.1.08.04.0A 2.1.08.04.0B
2.1.08.08	Capillary Effects in EBS	- Wicking	EBS (FLOW)	Include	1 (resaturation of excavation		2.1.08.06.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.08.09	Influx/Seepage Into the EBS	 Water influx rate (spatial and temporal distribution) [see also Open Boreholes in 1.1.01.01, Thermal Effects on Flow in EBS in 2.1.11.10, Flow Through Host Rock in 2.2.08.01, Effects of Excavation on Flow in 2.2.08.04] 	EBS-NF	Include	1 (resaturation of excavation as part of closure and healing of EDZ)		2.1.08.01.0A
2.1.09.00	1.09. CHEMICAL PROCESSES - CHEMISTRY						
2.1.09.01	Chemistry of Water Flowing into the Repository	 Chemistry of influent water (spatial and temporal distribution) [See also Chemistry in Host Rock 2.2.09.01] 	EBS-NF	Include	1		2.2.08.12.0A 2.1.08.01.0A
2.1.09.02	Chemical Characteristics of Water in Waste Packages	 Water composition (radionuclides, dissolved species,) Initial void chemistry (air / gas) Water chemistry (pH, ionic strength, pCO₂,) Reduction-oxidation potential Reaction kinetics Influent chemistry (from tunnels and/or backfill) [see also Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] Evolution of water chemistry / interaction with waste packages 	WF-WP	Include	1		2.1.09.01.0B 2.1.02.09.0A 2.2.08.12.0B 2.1.09.06.0A 2.1.09.07.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.09.03	Chemical Characteristics of Water in Backfill	 Water composition (radionuclides, dissolved species,) Water chemistry (pH, ionic strength, pCO₂,) Reduction-oxidation potential Reaction kinetics Influent chemistry (from tunnels and/or waste package) [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Tunnels in 2.1.09.04] Evolution of water chemistry / interaction with backfill 	BUFF	Include	1		2.1.04.02.0A 2.1.09.01.0A 2.1.09.06.0B 2.1.09.07.0B
2.1.09.04	Chemical Characteristics of Water in Drifts	 Water composition (radionuclides, dissolved species,) Water chemistry (pH, ionic strength, pCO₂,) Reduction-oxidation potential Reaction kinetics Influent chemistry (from near-field host rock) Initial chemistry (from construction / emplacement) [see also Chemical Effects from Preclosure in 1.1.02.01, Chemistry of Water Flowing in 2.1.09.01, Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03] Evolution of water chemistry / interaction with seals, liner/rock reinforcement materials, waste package support materials 	BUFF-SL	Include	1	A2.2.4	2.1.09.01.0A 2.1.09.06.0B 2.1.09.07.0B

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.09.05	Chemical Interaction of Water with Corrosion Products - In Waste Packages - In Backfill - In Drifts	 Corrosion product formation and composition (waste form, waste package internals, waste package) Evolution of water chemistry in waste packages, in backfill, and in tunnels [contributes to Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] 	WF-WP	Include	1	B1.2 B1.2.1	2.1.09.02.0A
2.1.09.06	Chemical Interaction of Water with Backfill - On Waste Packages - In Backfill - In Drifts	 Backfill composition and evolution (bentonite, crushed rock,) Evolution of water chemistry in backfill, and in tunnels Enhanced degradation of waste packages (crevice formation) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04, Localized Corrosion of WPs in 2.1.03.04] 	BUFF	Include	1	B1.2 B1.2.1	2.1.04.02.0A
2.1.09.07	Chemical Interaction of Water with Liner / Rock Reinforcement and Cementitious Materials in EBS - In Backfill - In Drifts	 Liner composition and evolution (concrete, metal,) Rock reinforcement material composition and evolution (grout, rock bolts, mesh,) Other cementitious materials composition and evolution Evolution of water chemistry in backfill, and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] 	SL	Include	1		2.1.06.01.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.09.08	Chemical Interaction of Water with Other EBS Components - In Waste Packages - In Drifts	 Seals composition and evolution Waste Package Support composition and evolution (concrete, metal,) Other EBS components (other metals (copper),) Evolution of water chemistry in backfill, and in tunnels [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] 	SL	Include	1	B1.2 B1.2.1	2.1.06.05.0D 2.1.03.09.0A
2.1.09.09	Chemical Effects at EBS Component Interfaces	 Component-to-component contact (chemical reactions) Consolidation of EBS components 	EBS (CHEM)	Include	1	B1.2 B1.2.1	2.1.06.07.0A 2.1.08.15.0A
2.1.09.10	Chemical Effects of Waste- Rock Contact	 Waste-to-host rock contact (chemical reactions) Component-to-host rock contact (chemical reactions) 	EBS (CHEM)	Include	1	B1.2 B1.2.1	2.1.09.11.0A 2.2.01.02.0B
2.1.09.11	Electrochemical Effects in EBS	- Enhanced metal corrosion	EBS (CHEM)	Include	1		2.1.09.09.0A 2.1.09.27.0A
2.1.09.12	Chemical Effects of Drift Collapse	 Evolution of water chemistry in backfill and in drifts (from altered seepage, from altered thermal-hydrology) [contributes to Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] 	EBS-NF	Include	1		1.2.03.02.0E
2.1.09.13	Radionuclide Speciation and Solubility in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Dissolved concentration limits Limited dissolution due to inclusion in secondary phase Enhanced dissolution due to alpha recoil [controlled by Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] 	EBS (CHEM)	Include	1		2.1.09.04.0A 2.1.09.10.0A 2.1.02.04.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.09.50	1.09. CHEMICAL PROCESSES - TRANSPORT						
2.1.09.51	Advection of Dissolved Radionuclides in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Flow pathways and velocity Advective properties (porosity, tortuosity) Dispersion Saturation [see also Gas Phase Transport in 2.1.12.03] 	EBS (TRAN)	Exclude	2 Most clay/shale site would have minimal advection but would be important aspect of site characterization		2.1.09.08.0B 2.1.04.09.0A 2.1.09.27.0A
2.1.09.52	Diffusion of Dissolved Radionuclides in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Gradients (concentration, chemical potential) Diffusive properties (diffusion coefficients) Flow pathways and velocity Saturation 	EBS (TRAN)	Include	1		2.1.09.08.0A 2.1.04.09.0A 2.1.09.27.0A
2.1.09.53	Sorption of Dissolved Radionuclides in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Surface complexation properties Mineral surface areas Ion exchange Flow pathways and velocity Saturation [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04] 	EBS (TRAN)	Include	1	A2.2.3 A2.2.7 A2.2.8	2.1.09.05.0A 2.1.04.09.0A 2.1.09.27.0A
2.1.09.54	Complexation in EBS	 Formation of organic complexants (humates, fulvates, organic waste) Enhanced transport of radionuclides associated with organic complexants [see also Degradation of Organics in Waste in 2.1.02.03] 	EBS (TRAN)	Include	1	A2.2.2 B1.2.2	2.1.09.13.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.09.55	Formation of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Formation of intrinsic colloids Formation of pseudo colloids (host rock fragments, waste form fragments, corrosion products, microbes) Formation of co-precipitated colloids Sorption/attachment of radionuclides to colloids (clay, silica, waste form, FeOx, microbes) 	EBS (TRAN)	Exclude	2 Clay/shale formations would usually prevent colloid transport but would be important aspect of site characterization		2.1.09.15.0A 2.1.09.16.0A 2.1.09.17.0A 2.1.09.18.0A 2.1.09.25.0A
2.1.09.56	Stability of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Chemical stability of attachment (dependent on water chemistry) Mechanical stability of colloid (dependent on colloid size, gravitational settling) 	EBS (TRAN)	Exclude	2		2.1.09.23.0A 2.1.09.26.0A 2.1.09.21.0A
2.1.09.57	Advection of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Flow pathways and velocity Advective properties (porosity, tortuosity) Dispersion Saturation Colloid concentration 	EBS (TRAN)	Exclude	1		2.1.09.19.0B 2.1.04.09.0A
2.1.09.58	Diffusion of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Drift	 Gradients (concentration, chemical potential) Diffusive properties (diffusion coefficients) Flow pathways and velocity Saturation Colloid concentration 	EBS (TRAN)	Exclude	1		2.1.09.24.0A 2.1.04.09.0A
2.1.09.59	Sorption of Colloids in EBS - In Waste Form - In Waste Package - In Backfill - In Tunnel	 Surface complexation properties Flow pathways and velocity Saturation Colloid concentration [see also Chemistry in Waste Packages in 2.1.09.02, Chemistry in Backfill in 2.1.09.03, Chemistry in Tunnels in 2.1.09.04]	EBS (TRAN)	Exclude	1		2.1.09.19.0A 2.1.04.09.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.09.60	Sorption of Colloids at Air- Water Interface in EBS		EBS (TRAN)	Exclude	1		2.1.09.22.0A
2.1.09.61	Filtration of Colloids in EBS	 Physical filtration (dependent on flow pathways, colloid size)- Electrostatic filtration 	EBS (TRAN)	Exclude	1 Included if colloid formation (2.1.09.55) included		2.1.09.20.0A 2.1.09.21.0A
2.1.09.62	Radionuclide Transport Through Liners and Seals	 Advection Dispersion Diffusion Sorption [contributes to Radionuclide release from EBS in 2.1.09.63] 	SL	Include	1		2.1.05.02.0A
2.1.09.63	Radionuclide Release from the EBS - Dissolved - Colloidal - Gas Phase	 Spatial and temporal distribution of releases to the host rock (due to varying flow pathways and velocities, varying component degradation rates, varying transport properties) [contributions from Dissolved in 2.1.09.51/52/53, Colloidal in 2.1.09.57/58/59, Gas Phase in 2.1.12.03, Liners and Seals in 2.1.09.62] 	EBS-NF	Include	1		2.2.07.06.0A 2.2.07.06.0B

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.10.00	1.10. BIOLOGICAL PROCESSES						
2.1.10.01	Microbial Activity in EBS - Natural - Anthropogenic	 Effects on corrosion Formation of complexants Formation of microbial colloids Formation of biofilms Biodegradation Biomass production Bioaccumulation [see also Microbiallly Influenced Corrosion in 2.1.03.06, Complexation in EBS in 2.1.09.54, Radiological Mutation of Microbes in 2.1.13.03] 	EBS (BIO)	Include	1	B7	2.1.10.01.0A
2.1.11.00	1.11. THERMAL PROCESSES						
2.1.11.01	Heat Generation in EBS	 Heat transfer (spatial and temporal distribution of temperature and relative humidity) [see also Thermal-Hydrologic Effects from Preclosure in 1.1.02.03, Waste Inventory in 2.1.01.01] 	EBS (T- H-C)	Include	1		2.1.11.01.0A 2.1.11.02.0A
2.1.11.02	Exothermic Reactions in EBS	- Oxidation of SNF - Hydration of concrete	EBS (MECH)	Include	1		2.1.11.03.0A
2.1.11.03	Effects of Backfill on EBS Thermal Environment	- Thermal blanket - Condensation - Thermal properties	BUFF	Include	1	B2.2	2.1.04.04.0A
2.1.11.04	Effects of Drift Collapse on EBS Thermal Environment	- Thermal blanket - Condensation	EBS-NF	Include	1 Part of closure and healing of EDZ		1.2.03.02.0D

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.11.05	Effects of Influx (Seepage) on Thermal Environment	- Temperature and relative humidity (spatial and temporal distribution) [see also Influx/Seepage into EBS in 2.1.08.09]	EBS-NF	Include	1 Part of resaturation of EDZ		2.1.08.01.0B 2.1.08.01.0A
2.1.11.06	Thermal-Mechanical Effects on Waste Form and In-Package EBS Components	- Alteration - Cracking - Thermal expansion / stress	WF	Include	1 Part of closure and healing of EDZ		2.1.11.05.0A
2.1.11.07	Thermal-Mechanical Effects on Waste Packages	 Thermal sensitization / phase changes Cracking Thermal expansion / stress / creep 	WP	Include	1		2.1.07.05.0A 2.1.11.06.0A 2.1.11.07.0A
2.1.11.08	Thermal-Mechanical Effects on Backfill	- Alteration - Cracking - Thermal expansion / stress	BUFF	Include	1		2.1.11.07.0A 2.1.04.04.0A
2.1.11.09	Thermal-Mechanical Effects on Other EBS Components - Seals - Liner / Rock Reinforcement Materials - Waste Package Support Structure	 Alteration Cracking Thermal expansion / stress Thermal properties 	SL	Include	1	B2.2	2.1.11.07.0A
2.1.11.10	Thermal Effects on Flow in EBS	 Altered influx/seepage Altered saturation / relative humidity (dry-out, resaturation) Condensation 	EBS (T- H)	Include	1		2.1.08.03.0A 2.1.08.11.0A 2.1.11.09.0A
2.1.11.11	Thermally-Driven Flow (Convection) in EBS	- Convection	EBS (T- H)	Include	1		2.1.11.09.0B 2.1.11.09.0C
2.1.11.12	Thermally-Driven Buoyant Flow / Heat Pipes in EBS	- Vapor flow	EBS (T- H)	Include	1		2.2.10.10.0A
2.1.11.13	Thermal Effects on Chemistry and Microbial Activity in EBS		EBS (T- C)	Include	1		2.1.11.08.0A
2.1.11.14	Thermal Effects on Transport in EBS	- Thermal diffusion (Soret effect) - Thermal osmosis	EBS (T- H-C)	Include	1		2.1.11.10.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.12.00	1.12. GAS SOURCES AND EFFECTS						
2.1.12.01	Gas Generation in EBS	 Repository Pressurization Mechanical Damage to EBS Components He generation from waste from alpha decay H₂ generation from waste package corrosion CO₂, CH₄, and H₂S generation from microbial degradation 	WF-WP	Include	1		2.1.12.01.0A 2.1.12.02.0A 2.1.12.03.0A 2.1.12.04.0A
2.1.12.02	Effects of Gas on Flow Through the EBS	- Two-phase flow - Gas bubbles [see also Buoyant Flow/Heat Pipes in 2.1.11.12]	EBS (FLOW)	Include	1		2.1.12.06.0A 2.1.12.07.0A
2.1.12.03	Gas Transport in EBS	- Gas phase transport - Gas phase release from EBS	EBS (TRAN)	Include	1	B6.4	2.1.12.07.0A 2.1.12.06.0A 2.2.10.10.0A
2.1.12.04	Gas Explosions in EBS	[see also Flammable Gas from Waste in 2.1.02.05]	EBS (MECH)	Exclude	1		2.1.12.08.0A
2.1.13.00	1.13. RADIATION EFFECTS						
2.1.13.01	Radiolysis - In Waste Package - In Backfill - In Drift	 Gas generation Altered water chemistry 	EBS (CHEM)	Exclude	1		2.1.13.01.0A
2.1.13.02	Radiation Damage to EBS Components - Waste Form - Waste Package - Backfill - Other EBS Components	 Enhanced waste form degradation Enhanced waste package degradation Enhanced backfill degradation Enhanced degradation of other EBS components (liner/rock reinforcement materials, seals, waste support structure) 	EBS (MECH)	Exclude	1		2.1.13.02.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.1.13.03	Radiological Mutation of Microbes		EBS (BIO)	Exclude	1		2.1.13.03.0A
2.1.14.00	1.14. NUCLEAR CRITICALITY						
2.1.14.01	Criticality In-Package	- Formation of critical configuration	WF-WP	Exclude	1		2.1.14.15.0A 2.1.14.16.0A 2.1.14.21.0A 2.1.14.22.0A
2.1.14.02	Criticality in EBS or Near-Field	- Formation of critical configuration	EBS (TRAN)	Exclude	1		2.1.14.17.0A 2.1.14.23.0A
2.2.00.00	2. GEOLOGICAL ENVIRONMENT						
2.2.01.00	2.01. EXCAVATION DISTURBED ZONE (EDZ)						
2.2.01.01	Evolution of EDZ	 Size and extent, Structure and heterogeneities Geomechanical properties Hydraulic properties Flow pathways Chemical characteristics of groundwater in EDZ Radionuclide speciation and solubility in EDZ Thermal-mechanical effects Thermal-chemical alteration Thermal-hydrologic-mechanical effects Oxidation of the host rock Geomechanical stability [see also Mechanical Effects of Excavation in 1.1.02.02] 	EDZ	Include	1 Usually short-lived in clay/shale	B1.1 B2.3 B3.1 B3.2 B3.4 B4.1 B4.2 B5.1 B5.2 B5.3 C2.4	2.2.01.04.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.02.00	2.02. HOST ROCK						
2.2.02.01	Stratigraphy and Properties of Host Rock	 Rock units Thickness, lateral extent, heterogeneities, discontinuities, contacts Geomechanical properties Flow pathways [see also Fractures in 2.2.05.01 and Faults in 2.2.05.02] 	HR	Include	1	A1.1.1 A1.1.2 B3.4	2.2.03.01.0A 2.2.03.02.0A
2.2.03.00	2.03. OTHER GEOLOGIC UNITS						
2.2.03.01	Stratigraphy and Properties of Other Geologic Units (Non- Host-Rock) - Confining units - Aquifers	 Rock units Thickness, lateral extent, heterogeneities, discontinuities, contacts Physical properties Flow pathways [see also Fractures in 2.2.05.01 and Faults in 2.2.05.02] 	GU	Include	1	A1.1.1 A1.1.2	2.2.03.01.0A 2.2.03.02.0A
2.2.05.00	2.05. FLOW AND TRANSPORT PATHWAYS						
2.2.05.01	Fractures - Host Rock	 Flow and transport properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01] 	GEO (FLOW)	Exclude	1	A1.1.5	1.2.02.01.0A 2.2.07.13.0A
2.2.05.02	Fractures - Other Geologic Units	 Flow and transport properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01] 	GEO (FLOW)	Exclude?	1 Dependent on location of clay/shale site		1.2.02.01.0A 2.2.07.13.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.05.03	Faults - Host Rock	 Flow and transport properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01] 	GEO (FLOW)	Exclude?	1 Dependent on location of clay/shale site		1.2.02.02.0A 2.2.07.13.0A
2.2.05.04	Faults - Other Geologic Units	- Flow and transport properties [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01]	GEO (FLOW)	Exclude?	1 Dependent on location of clay/shale site		1.2.02.02.0A 2.2.07.13.0A
2.2.05.05	Alteration and Evolution of Geosphere Flow Pathways - Host Rock - Other Geologic Units	 Changes In rock properties Changes in faults Changes in fractures Plugging of flow pathways Changes in saturation [see also Stratigraphy and Properties in 2.2.02.01 and 2.2.03.01, Fractures in 2.2.05.01, and Faults in 2.2.05.02] [see also Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07] 	GEO (FLOW)	Exclude	1 Possibly relevant in advective dominated portion of system	C3.3	2.2.12.00.0A 2.2.12.00.0B

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.07.00	2.07. MECHANICAL PROCESSES						
2.2.07.01	Mechanical Effects on Host Rock	 From subsidence From salt creep From clay deformation From granite deformation (rockfall / drift collapse into tunnels) Chemical precipitation / dissolution [see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07] 	HR	Include	2		2.2.06.04.0A 2.2.06.05.0A
2.2.07.02	Mechanical Effects on Other Geologic Units	 From subsidence Chemical precipitation / dissolution [see also Subsidence in 1.2.02.01, Thermal-Mechanical Effects in 2.2.11.06 and Thermal-Chemical Alteration in 2.2.11.07] 	GU	Exclude?	1 Dependent on location of clay/shale site		2.2.06.04.0A
2.2.07.03	Stress regime	-	GU	Include	1 Part of site characterization	C2.5	

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.08.00	2.08. HYDROLOGIC PROCESSES						
2.2.08.01	Flow Through the Host Rock	 Saturated flow Fracture flow / matrix imbibition Unsaturated flow (fingering, capillarity, episodicity, perched water) Preferential flow pathways Density effects on flow Flow pathways out of Host Rock Paleo-hydrogeology [see also Influx/Seepage into EBS in 2.1.08.09, Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02] 	HR	Include	1	A1.1.4 A1.1.5 A3.1 C1.1.1	2.2.07.02.0A 2.2.07.03.0A 2.2.07.04.0A 2.2.07.05.0A 2.2.07.07.0A 2.2.07.08.0A 2.2.07.09.0A 2.2.07.12.0A
2.2.08.02	Flow Through the Other Geologic Units - Confining units - Aquifers	 Saturated flow Fracture flow / matrix imbibition Unsaturated flow (fingering, capillarity, episodicity, perched water) Preferential flow pathways Density effects on flow Flow pathways out of Other Geologic Units Paleo-hydrogeology [see also Alteration of Flow Pathways in 2.2.05.03, Thermal Effects on Flow in 2.2.11.01, Effects of Gas on Flow in 2.2.12.02] 	GU	Include	1	A1.1.4 A1.1.6 A3.1 C1.1.1	2.2.07.02.0A 2.2.07.03.0A 2.2.07.04.0A 2.2.07.05.0A 2.2.07.07.0A 2.2.07.08.0A 2.2.07.09.0A 2.2.07.12.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.08.03	Effects of Recharge on Geosphere Flow - Host Rock - Other Geologic Units	- Infiltration rate - Water table rise/decline [see also Infiltration in 2.3.08.03]	GEO-BIO	Include	1		1.3.07.01.0A 1.3.07.02.0A 1.3.07.02.0B
2.2.08.04	Effects of Repository Excavation on Flow Through the Host Rock	 Saturated flow (flow sink) Unsaturated flow (capillary diversion, drift shadow) Influx/Seepage into EBS (film flow, enhanced seepage) [see also Influx/Seepage into EBS in 2.1.08.09] 	EDZ-HR	Include	1		2.1.08.02.0A 2.2.07.18.0A 2.2.07.20.0A 2.2.07.21.0A
2.2.08.05	Condensation Forms in Host Rock	 Condensation cap Shedding [see also Thermal Effects on Flow in Geosphere in 2.2.11.01] 	HR	Exclude	1		2.2.07.10.0A
2.2.08.06	Flow Through EDZ	 Saturated / Unsaturated flow Fracture / Matrix flow 	EDZ	Include	1		2.2.01.03.0A
2.2.08.07	Mineralogic Dehydration	 Dehydration reactions release water and may lead to volume changes 	GEO (FLOW)	Include	1		2.2.10.14.0A
2.2.08.08	Groundwater Discharge to Biosphere Boundary	 Surface discharge (water table, capillary rise, surface water) Flow across regulatory boundary 	GEO-BIO	Include	1		2.2.08.11.0A 2.3.11.04.0A
2.2.08.09	Groundwater Discharge to Well	 Human use (drinking water, bathing water, industrial) Agricultural use (irrigation, animal watering) 	GEO-BIO	Include	1		1.4.07.02.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.00	2.09.CHEMICAL PROCESSES - CHEMISTRY						
2.2.09.01	Chemical Characteristics of Groundwater in Host Rock	 Water composition (radionuclides, dissolved species,) Water chemistry (temperature, pH, Eh, ionic strength) Reduction-oxidation potential Reaction kinetics Interaction with EBS Interaction with host rock Future changes [see also Chemistry in Tunnels in 2.1.09.04, Chemical Interactions and Evolution in 2.2.09.03] [contributes to Chemistry of Water Flowing into Repository in 2.1.09.01] 	HR	Include	1	C1.2.2	2.2.01.02.0B 2.2.08.01.0B
2.2.09.02	Chemical Characteristics of Groundwater in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	 Water composition (radionuclides, dissolved species,) Water chemistry (temperature, pH, Eh, ionic strength) Reduction-oxidation potential Reaction kinetics Interaction with other geologic units Future changes [see also Chemical Interactions and Evolution in 2.2.09.04]	GU	Include	1	C1.2.2	2.2.08.01.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.03	Chemical Interactions and Evolution of Groundwater in Host Rock	 Host rock composition and evolution (granite, clay, salt) Evolution of water chemistry in host rock Thermal effects on mineral stability Thermal effects on pore-water chemistry Chemical effects on density Interaction with EBS Reaction kinetics Mineral dissolution/precipitation Redissolution of precipitates after dry- out Paleo-hydrogeology Water residence times Redox buffering capacity of the host rock Chemical osmosis 	HR	Include	1	A3.1 A3.2 A3.3 B1.1.1 B2.1 B5.5 C1.1.1 C1.1.2	2.2.01.02.0B 2.2.07.14.0A 2.2.08.03.0B 2.2.08.04.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.04	Chemical Interactions and Evolution of Groundwater in Other Geologic Units (Non- Host-Rock) - Confining units - Aquifers	 Host rock composition and evolution (granite, clay, salt) Evolution of water chemistry in host rock Chemical effects on density Reaction kinetics Mineral dissolution/precipitation Recharge chemistry Paleo-hydrogeology Water residence times 	GU	Include	1	A3.1 A3.2 A3.3 C1.1.1 C1.1.2	2.2.07.14.0A 2.2.08.03.0A
		Geologic Units in 2.2.09.02]					
2.2.09.05	Radionuclide Speciation and Solubility in Host Rock	- Dissolved concentration limits [controlled by Chemistry in Host Rock in 2.2.09.01]	HR	Include	1		2.2.08.07.0B
2.2.09.06	Radionuclide Speciation and Solubility in Other Geologic Units (Non-Host-Rock) - Confining units - Aquifers	- Dissolved concentration limits [controlled by Chemistry in Other Geologic Units in 2.2.09.02]	GU	Include	1		2.2.08.07.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.50	2.09. CHEMICAL PROCESSES - TRANSPORT						
2.2.09.51	Advection of Dissolved Radionuclides in Host Rock	 Flow pathways and velocity Advective properties (porosity, tortuosity, wetted surface) Dispersion Matrix diffusion Saturation [see also Gas Phase Transport in 2.2.12.03] 	GEO (TRAN)	Exclude	2 Most clay/shale site would have minimal advection but would be important aspect of site characterization	A1.1 A2.1.3	2.2.07.15.0B 2.2.08.08.0B
2.2.09.52	Advection of Dissolved Radionuclides in Other Geologic Units (Non-Host- Rock) - Confining units - Aquifers	 Flow pathways and velocity Advective properties (porosity, tortuosity, wetted surface) Dispersion Matrix diffusion Saturation [see also Gas Phase Transport in 2.2.12.03] 	GEO (TRAN)	Include	1	A1.1 A2.1.3	2.2.07.15.0A 2.2.08.08.0A
2.2.09.53	Diffusion of Dissolved Radionuclides in Host Rock	 Gradients (concentration, chemical potential) Diffusive properties (diffusion coefficients) Connected matrix porosity Flow pathways and velocity Saturation Ion Exclusion Surface diffusion 	GEO (TRAN)	Include	1	A1.2.1 A1.2.2 A1.2.3 A1.2.4 A2.1.1 A2.1.2 A2.1.4 A.2.1.5	2.2.08.05.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.54	Diffusion of Dissolved Radionuclides in Other Geologic Units (Non-Host- Rock) - Confining units - Aquifers	 Gradients (concentration, chemical potential) Diffusive properties (diffusion coefficients) Connected matrix porosity Flow pathways and velocity Saturation Ion Exclusion Surface diffusion 	GEO (TRAN)	Include	1	A1.2.1 A1.2.2 A1.2.3 A1.2.4 A2.1.1 A2.1.2 A2.1.4 A.2.1.5	2.2.07.17.0A
2.2.09.55	Sorption of Dissolved Radionuclides in Host Rock	 Lithology, mineralogy of rocks Surface complexation properties Ion exchange Dissolution/precipitation of solid phases Solid solutions/co-precipitation Thermodynamic and kinetic data Mineral surface areas, fracture infills Flow pathways and velocity Saturation [see also Chemistry in Host Rock in 2.2.09.01]	GEO (TRAN)	Include	1	A2.2.1 A2.2.3 A2.2.5 A2.2.6 A2.2.7 A2.2.8 A2.2.9	2.2.08.09.0B
2.2.09.56	Sorption of Dissolved Radionuclides in Other Geologic Units (Non-Host- Rock) - Confining units - Aquifers	 Lithology, mineralogy of rocks Surface complexation properties Ion exchange Dissolution/precipitation of solid phases Solid solutions/co-precipitation thermodynamic and kinetic data Mineral surface areas, fracture infills Flow pathways and velocity Saturation [see also Chemistry in Host Rock in 2.2.09.01]	GEO (TRAN)	Include	1	A2.2.1 A2.2.3 A2.2.5 A2.2.6 A2.2.7 A2.2.8 A2.2.9	2.2.08.09.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.57	Complexation in Host Rock	 Presence of organic complexants (humates, fulvates, carbonates,) Enhanced transport of radionuclides associated with organic complexants 	GEO (TRAN)	Include?	2 Organic content clay/shale would be important aspect of site characterization	A2.2.2	2.1.09.21.0C 2.2.08.06.0B
2.2.09.58	Complexation in Other Geologic Units (Non-Host- Rock) - Confining units - Aquifers	 Presence of organic complexants (humates, fulvates, carbonates,) Enhanced transport of radionuclides associated with organic complexants 	GEO (TRAN)	Exclude?	2 important aspect of site characterization	A2.2.2	2.1.09.21.0B 2.2.08.06.0A
2.2.09.59	Colloidal Transport in Host Rock	 Flow pathways and velocity Saturation Advection Dispersion Diffusion Sorption Colloid concentration 	GEO (TRAN)	Exclude	1	A1.3	2.2.08.10.0B
2.2.09.60	Colloidal Transport in Other Geologic Units (Non-Host- Rock) - Confining units - Aquifers	 Flow pathways and velocity Saturation Advection Dispersion Diffusion Sorption Colloid concentration 	GEO (TRAN)	Exclude	1 Could be important in advection dominated portion of system	A1.3	2.2.08.10.0A
2.2.09.61	Radionuclide Transport Through EDZ	- Advection - Dispersion - Diffusion - Ion Exclusion - Sorption	EDZ	Include	1 Transport in EDZ would be short- term prior to healing	A1.2.3 A2.1.4	2.2.01.05.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.62	Dilution of Radionuclides in Groundwater - Host Rock - Other Geologic Units	 Mixing with uncontaminated groundwater Mixing at withdrawal well [see also Groundwater Discharge to Well in 2.2.08.09] 	GEO (TRAN)	Include	1		2.2.07.16.0A
2.2.09.63	Dilution of Radionuclides with Stable Isotopes - Host Rock - Other Geologic Units	 Mixing with stable and/or naturally occurring isotopes of the same element 	GEO (TRAN)	Include?	1 Could be important for some radioisotopes such as ¹²⁹ 1		3.2.07.01.0A
2.2.09.64	Radionuclide Release from Host Rock - Dissolved - Colloidal - Gas Phase	 Spatial and temporal distribution of releases to the Other Geologic Units (due to varying flow pathways and velocities, varying transport properties) [contributions from Dissolved in 2.2.09.51/53/55, Colloidal in 2.2.09.59, Gas Phase in 2.2.12.03, EDZ in 2.2.09.61] 	HR-GU	Include	1		

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.09.65	Radionuclide Release from Other Geologic Units - Dissolved - Colloidal - Gas Phase	 Spatial and temporal distribution of releases to the Biosphere (due to varying flow pathways and velocities, varying transport properties) [see also Groundwater Discharge to Biosphere Boundary in 2.2.08.08, Groundwater Discharge to Well in 2.2.08.09, Recycling of Accumulated Radionuclides in 2.3.09.55] [contributions from Dissolved in 2.2.09.52/54/56, Colloidal in 2.2.09.60, Gas Phase in 2.2.12.03] 	GEO-BIO	Include	1		1.4.07.02.0A 2.2.08.11.0A 2.3.11.04.0A 2.3.13.04.0A
2.2.10.00	2.10. BIOLOGICAL PROCESSES						
2.2.10.01	Microbial Activity in Host Rock	 Formation of complexants Formation and stability of microbial colloids Biodegradation Bioaccumulation [see also Complexation in Host Rock in 2.2.09.57] 	HR	Exclude	1	Β7	2.2.09.01.0B
2.2.10.02	Microbial Activity in Other Geologic Units (Non-Host- Rock) - Confining units - Aquifers	 Formation of complexants Formation and stability of microbial colloids Biodegradation Bioaccumulation [see also Complexation in Other Geologic Units in 2.2.09.58] 	GU	Exclude	1	Β7	2.2.09.01.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.11.00	2.11. THERMAL PROCESSES						
2.2.11.01	Thermal Effects on Flow in Geosphere - Repository-Induced - Natural Geothermal	 Thermal properties Altered saturation / relative humidity (dry-out, resaturation) Altered gradients, density, and/or flow pathways Vapor flow Condensation 	GEO (T- H)	Include	1	B2.2	1.2.06.00.0A 2.2.07.11.0A 2.2.10.01.0A 2.2.10.03.0A 2.2.10.03.0B 2.2.10.11.0A 2.2.10.12.0A 2.2.10.12.0A 2.2.10.13.0A
2.2.11.02	Thermally-Driven Flow (Convection) in Geosphere	- Convection	GEO (T- H)	Include	1		2.2.10.02.0A
2.2.11.03	Thermally-Driven Buoyant Flow / Heat Pipes in Geosphere	- Vapor flow	GEO (T- H)	Include	1		2.2.10.10.0A
2.2.11.04	Thermal Effects on Chemistry and Microbial Activity in Geosphere	 Mineral precipitation / dissolution Altered solubility [contributes to Chemistry in 2.2.09.01 and 2.2.09.02] 	GEO (T- C)	Exclude	1		2.2.10.06.0A 2.2.10.08.0A
2.2.11.05	Thermal Effects on Transport in Geosphere	 Thermal diffusion (Soret effect—Off diagonal Onsager process) Thermal osmosis 	GEO (T- H-C)	Exclude	1	B5.4	
2.2.11.06	Thermal-Mechanical Effects on Geosphere	 Thermal expansion / compression Altered properties of fractures, faults, rock matrix 	GEO (T- M)	Include	1		2.2.01.02.0A 2.2.10.04.0A 2.2.10.04.0B 2.2.10.05.0A
2.2.11.07	Thermal-Chemical Alteration of Geosphere	 Mineral precipitation / dissolution Altered properties of fractures, faults, rock matrix Alteration of minerals / volume changes Formation of near-field chemically altered zone (rind) 	GEO (T- C-M)	Include	1		2.1.09.12.0A 2.2.10.06.0A 2.2.10.07.0A 2.2.10.08.0A 2.2.10.09.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.2.12.00	2.12. GAS SOURCES AND EFFECTS						
2.2.12.01	Gas Generation in Geosphere	 Degassing (clathrates, deep gases) Microbial degradation of organics 	GEO (FLOW)	Exclude	1		2.2.11.01.0A 2.2.11.02.0A
2.2.12.02	Effects of Gas on Flow Through the Geosphere	 Altered gradients and/or flow pathways Vapor/air flow Two-phase flow Gas bubbles [see also Buoyant Flow/Heat Pipes in 2.2.11.03] 	GEO (FLOW)	Include	1	B6.1 B6.2 B6.3	2.2.10.11.0A 2.2.11.01.0A 2.2.11.02.0A
2.2.12.03	Gas Transport in Geosphere	 Gas phase transport Gas phase release from Geosphere 	GEO (TRAN)	Include	1	B6.2 B6.3 B6.4	2.2.11.03.0A
2.2.14.00	2.14. NUCLEAR CRITICALITY						
2.2.14.01	Criticality in Far-Field	- Formation of critical configuration	GEO (TRAN)	Exclude	1		2.2.14.09.0A 2.2.14.11.0A
2.2.16.00	2.16 Undetected Features						
2.2.16.01	2.16 Undetected Geologic Features			Exclude?	2 Undetected features mostly irrelevant for diffusion dominated systems; might be important for parts of disposal system dominated by advection	A1.1.3	

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.3.00.00	3. SURFACE ENVIRONMENT						
2.3.01.00	3.01. SURFACE CHARACTERISTICS						
2.3.01.01	Topography and Surface Morphology	- Recharge and discharge areas	BIO	Include	1		2.3.01.00.0A
2.3.02.01	Surficial Soil Type	- Physical and chemical attributes	BIO	Include	1		2.3.02.01.0A
2.3.04.01	Surface Water	 Lakes, rivers, springs Dams, reservoirs, canals, pipelines Coastal and marine features Water management activities 	BIO	Exclude	1		1.4.07.01.0A 2.3.06.00.0A
2.3.05.01	Biosphere Characteristics	 Climate Soils Flora and fauna Microbes Evolution of biosphere (natural, anthropogenic – e.g., acid rain) [see also Climate in 1.3.01.01, Surficial Soil Type in 2.3.02.01, Microbial Activity in 2.3.10.01] 	BIO	Include	1		2.3.13.01.0A
2.3.07.00	3.07. MECHANICAL PROCESSES						
2.3.07.01	Past and Future Erosion	 Weathering Denudation Subsidence [see also Subsidence in 1.2.02.01, Periglacial Effects in 1.3.04.01, Glacial Effects in 1.3.05.01, Surface Runoff in 2.3.08.02, and Soil and Sediment Transport in 2.3.09.53]	BIO (MECH)	Exclude	1	C2.6 C3.1 C3.2	1.2.07.01.0A 2.2.06.04.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.3.07.02	Past and Future Deposition	- burial	BIO (MECH)	Exclude	1	C1.1.3 C2.6 C3.1 C3.2	1.2.07.02.0A
2.3.07.03	Animal Intrusion into Repository		BIO (MECH)	Exclude	1		2.3.09.01.0A
2.3.08.00	3.08. HYDROLOGIC PROCESSES						
2.3.08.01	Precipitation	- Spatial and temporal distribution [see also Climate Change in 1.3.01.01] [contributes to Infiltration in 2.3.08.03]	BIO (FLOW)	Include	1		2.3.11.01.0A
2.3.08.02	Surface Runoff and Evapotranspiration	 Runoff, impoundments, flooding, increased recharge Evaporation Transpiration (root uptake) [see also Climate Change in 1.3.01.01, Erosion in 2.3.07.01] [contributes to Infiltration in 2.3.08.03] 	BIO (FLOW)	Include	1		2.3.11.02.0A 2.2.06.04.0A
2.3.08.03	Infiltration and Recharge	 Spatial and temporal distribution Effect on hydraulic gradient Effect on water table elevation [see also Topography in 2.3.01.01, Surficial Soil Type in 2.3.01.02] [contributes to Effects of Recharge in 2.2.08.03] 	BIO (FLOW)	Include	1		2.3.11.03.0A

Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
3.09. CHEMICAL PROCESSES - CHEMISTRY						
Chemical Characteristics of Soil and Surface Water	 Altered recharge chemistry (natural) Altered recharge chemistry (anthropogenic – e.g., acid rain) [contributes to Chemical Evolution of Groundwater in 2.2.09.04] 	BIO (CHEM)	Exclude	1		1.4.01.03.0A 1.4.06.01.0A
Radionuclide Speciation and Solubility in Biosphere	- Dissolved concentration limits	BIO (CHEM)	Exclude	1		2.2.08.07.0C
Radionuclide Alteration in Biosphere	 Altered physical and chemical properties Isotopic dilution 	BIO (CHEM)	Exclude	1 (isotopic dilution would more likely be included in geosphere transport)		2.3.13.02.0A 3.2.07.01.0A
3.09. CHEMICAL PROCESSES - TRANSPORT						
Atmospheric Transport Through Biosphere	 Radionuclide transport in air, gas, vapor, particulates, aerosols Processes include: wind, plowing, irrigation, degassing, saltation, precipitation 	BIO (TRAN)	Include	1		3.2.10.00.0A
Surface Water Transport Through Biosphere	 Radionuclide transport and mixing in surface water Processes include: lake mixing, river flow, spring discharge, aeration, sedimentation, dilution [see also Surface Water in 2.3.04.01] 	BIO (TRAN)	Exclude	1		2.3.04.01.0A
	3.09. CHEMICAL PROCESSES - CHEMISTRY Chemical Characteristics of Soil and Surface Water Radionuclide Speciation and Solubility in Biosphere Radionuclide Alteration in Biosphere 3.09. CHEMICAL PROCESSES - TRANSPORT Atmospheric Transport Through Biosphere Surface Water Transport	3.09. CHEMICAL PROCESSES - CHEMISTRY - Chemical Characteristics of Soil and Surface Water - Altered recharge chemistry (natural) - Altered recharge chemistry (anthropogenic – e.g., acid rain) Radionuclide Speciation and Solubility in Biosphere - Dissolved concentration limits Radionuclide Alteration in Biosphere - Altered physical and chemical properties 3.09. CHEMICAL PROCESSES - TRANSPORT - Altered physical and chemical properties Atmospheric Transport Through Biosphere - Radionuclide transport in air, gas, vapor, particulates, aerosols Surface Water Transport Through Biosphere - Radionuclide transport and mixing in surface water Surface Water Transport Through Biosphere - Radionuclide transport and mixing in surface water	3.09. CHEMICAL PROCESSES - CHEMISTRY- Altered recharge chemistry (natural) - Altered recharge chemistry (natural) - Altered recharge chemistry (anthropogenic – e.g., acid rain)BIO (CHEM)Radionuclide Speciation and Solubility in Biosphere- Dissolved concentration limitsBIO (CHEM)Radionuclide Alteration in Biosphere- Altered physical and chemical properties - Isotopic dilutionBIO (CHEM)3.09. CHEMICAL PROCESSES - TRANSPORT- Altered physical and chemical properties - Isotopic dilutionBIO (CHEM)3.09. CHEMICAL PROCESSES - TRANSPORT- Radionuclide transport in air, gas, vapor, particulates, aerosols - Processes include: wind, plowing, irrigation, degassing, saltation, precipitationBIO (TRAN)Surface Water Transport Through Biosphere- Radionuclide transport and mixing in surface water - Processes include: lake mixing, river flow, spring discharge, aeration, sedimentation, dilutionBIO (TRAN)	PhenomenaAssociated ProcessesDomainScreening Decision3.09. CHEMICAL PROCESSES - CHEMISTRYChemical Characteristics of Soil and Surface Water- Altered recharge chemistry (natural) - Altered recharge chemistry (anthropogenic – e.g., acid rain)BIO (CHEM)ExcludeRadionuclide Speciation and Solubility in Biosphere- Dissolved concentration limitsBIO (CHEM)ExcludeRadionuclide Alteration in Biosphere- Altered physical and chemical properties - Isotopic dilutionBIO (CHEM)Exclude3.09. CHEMICAL PROCESSES - TRANSPORT- Altered physical and chemical properties - Isotopic dilutionBIO (CHEM)Exclude3.09. CHEMICAL PROCESSES - TRANSPORT- Radionuclide transport in air, gas, vapor, particulates, aerosols - Processes include: wind, plowing, irrigation, degassing, saltation, precipitationBIO (TRAN)IncludeSurface Water Transport Through Biosphere- Radionuclide transport and mixing in surface water - Processes include: lake mixing, river flow, spring discharge, aeration, sedimentation, dilutionBIO (TRAN)Exclude	PhenomenaAssociated ProcessesDomainScreening DecisionLevel of Effort3.09. CHEMICAL PROCESSES - CHEMISTRYChemical Characteristics of Soil and Surface WaterAltered recharge chemistry (natural) BIO (CHEM)Exclude1Radionuclide Speciation and Solubility in Biosphere-Dissolved concentration limitsBIO (CHEM)Exclude1Radionuclide Alteration in Biosphere-Dissolved concentration limitsBIO (CHEM)Exclude1Radionuclide Alteration in BiosphereAltered physical and chemical properties -Isotopic dilutionBIO (CHEM)Exclude13.09. CHEMICAL PROCESSES - TRANSPORTAltered physical and chemical properties -Isotopic dilutionBIO (CHEM)Exclude13.09. CHEMICAL PROCESSES - TRANSPORTAltered physical and chemical properties -BIO (CHEM)Include1Atmospheric Transport Through BiosphereAltered physical and chemical processes include: wind, plowing, irrigation, degassing, saltation, precipitationBIO (TRAN)Include1Surface Water Transport Through BiosphereProcesses include: lake mixing, river flow, spring discharge, aeration, sedimentation, dilutionBIO (TRAN)Exclude1	PhenomenaAssociated ProcessesDomainScreening DecisionLevel of EffortMEA Clay FEP3.09. CHEMICAL PROCESSES - CHEMISTRYI

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.3.09.53	Soil and Sediment Transport Through Biosphere	 Radionuclide transport on soil and sediments Processes include: fluvial (runoff, river flow), eolian (wind), glaciation, bioturbation (animals) [see also Erosion in 2.3.07.01, Deposition in 2.3.07.02] 	BIO (TRAN)	Include	1		2.3.02.03.0A 2.3.09.01.0A
2.3.09.54	Radionuclide Accumulation in Soils	 Leaching/evaporation from discharge (well, groundwater upwelling) Deposition from atmosphere or water (irrigation, runoff) 	BIO (TRAN)	Include	1		2.3.02.02.0A
2.3.09.55	Recycling of Accumulated Radionuclides from Soils to Groundwater	[see also Radionuclide Release in 2.2.09.65]	BIO (TRAN)	Include	1		1.4.07.03.0A
2.3.10.00	3.10. BIOLOGICAL PROCESSES						
2.3.10.01	Microbial Activity in Biosphere	 Effect on biosphere characteristics Effect on transport through biosphere 	BIO (BIO)	Exclude	1		
2.3.11.00	3.11. THERMAL PROCESSES						
2.3.11.01	Effects of Repository Heat on Biosphere		BIO	Exclude	1		2.3.13.03.0A
2.4.00.00	4. HUMAN BEHAVIOR						
2.4.01.00	4.01. HUMAN CHARACTERISTICS						
2.4.01.01	Human Characteristics	 Physiology Metabolism Adults, children [contributes to Radiological Toxicity in 3.3.06.02] 	DOSE	Include	1		2.4.01.00.0A
2.4.01.02	Human Evolution	 Changing human characteristics Sensitization to radiation Changing lifestyle 	DOSE	Exclude	1		1.5.02.00.0A 3.3.06.02.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
2.4.04.00	4.04. LIFESTYLE						
2.4.04.01	Human Lifestyle	 Diet and fluid intake (food, water, tobacco/drugs, etc.) Dwellings Household activities Leisure activities [see also Land and Water Use in 2.4.08.01] [contributes to Ingestion in 3.3.04.01, Inhalation in 3.3.04.02, External Exposure in 3.3.04.03] 	DOSE	Include	1		2.4.04.01.0A 2.4.07.00.0A
2.4.08.00	4.08. LAND AND WATER USE						
2.4.08.01	Land and Water Use	 Agricultural (irrigation, plowing, fertilization, crop storage, greenhouses, hydroponics) Farms and Fisheries (feed, water, soil) Urban / Industrial (development, energy production, earthworks, population density) Natural / Wild (grasslands, forests, bush, surface water) 	DOSE	Include	1		2.4.08.00.0A 2.4.09.01.0B 2.4.09.02.0A 2.4.10.00.0A
2.4.08.02	Evolution of Land and Water Use	 New practices (agricultural, farming, fisheries) Technological developments Social developments (new/expanded communities) 	DOSE	Exclude	1		1.4.08.00.0A 1.4.09.00.0A 2.4.09.01.0A

UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
3.0.00.00	3. RADIONUCLIDE / CONTAMINANT FACTORS (BIOSPHERE)						
3.1.00.00	1. CONTAMINANT CHARACTERISTICS						
3.2.00.00	2. RELEASE / MIGRATION FACTORS						
3.3.00.00	3. EXPOSURE FACTORS						
3.3.01.00	3.01. RADIONUCLIDE / CONTAMINANT CONCENTRATIONS						
3.3.01.01	Radionuclides in Biosphere Media	 Soil Surface Water Air Plant Uptake Animal (Livestock, Fish) Uptake [contributions from Radionuclide Release from Geologic Units in 2.2.09.65, Transport Through Biosphere in 2.3.09.51/52/53/54/55] 	DOSE	Include	1		3.3.02.01.0A 3.3.02.02.0A 3.3.02.03.0A
3.3.01.02	Radionuclides in Food Products	 Diet and fluid sources (location, degree of contamination, dilution with uncontaminated sources) Foodstuff and fluid processing and preparation (water filtration, cooking techniques) [see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01] 	DOSE	Include	1		3.3.01.00.0A

Table B-1.	Generic Features, Events, and Processes List as Proposed by Used Fuel Disposition Campaign and Preliminary Screening Criteria
	(continued)

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UFD FEP Number	Phenomena	Associated Processes	Domain	Likely Screening Decision	Level of Effort	NEA Clay FEP	YMP FEP Database
3.3.01.03	Radionuclides in Non-Food Products	 Dwellings (location, building materials and sources, fuel sources) Household products (clothing and sources, furniture and sources, tobacco, pets) Biosphere media [see also Land and Water Use in 2.4.08.01, Radionuclides in Biosphere Media in 3.3.01.01] 	DOSE	Exclude	1		3.3.03.01.0A
3.3.04.00	3.04. EXPOSURE MODES						
3.3.04.01	Ingestion	 Food products Soil, surface water 	DOSE	Include	1		3.3.04.01.0A
3.3.04.02	Inhalation	 Gases and vapors Suspended particulates (dust, smoke, pollen) 	DOSE	Include	1		3.3.04.02.0A
3.3.04.03	External Exposure	 Non-Food products Soil, surface water 	DOSE	Include	1		3.3.04.03.0A
3.3.06.00	3.06. TOXICITY / EFFECTS						
3.3.06.01	Radiation Doses	 Exposure rates (ingestion, inhalation, external exposure) Dose conversion factors Gases and vapors Suspended particulates (dust, smoke, pollen) 	DOSE	Include	1		3.3.05.01.0A 3.3.08.00.0A
3.3.06.02	Radiological Toxicity and Effects	 Human health effects from radiation doses 	DOSE	Include	1		3.3.06.00.0A
3.3.06.03	Non-Radiological Toxicity and Effects	 Human health effects from non- radiological toxicity 	DOSE	Exclude	1		3.3.07.00.0A

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Distribution

1	MS0701	Marianne C. Walck	6700
1	MS0724	Jill M. Hruby	6000
1	MS0735	John A. Merson	6730
1	MS0736	John E. Kelly	6770
1	MS0751	Thomas Dewers	6735
1	MS0751	Katherine N. Gaither	6735
1	MS0751	Tom W. Pfeifle	6735
1	MS0754	Patrick V. Brady	6730
1	MS0754	Randall T. Cygan	6736
1	MS0754	James L. Krumhansl	6736
1	MS0754	Jeffery A. Greathouse	6736
5	MS0771	Stanley A. Orrell	6800
1	MS1369	Geoffrey A. Freeze	6784
1	MS1369	Robert P. Rechard	6782
1	MS1369	Robert J. MacKinnon	6782
1	MS1399	Palmer Vaughn	6786
5	MS1399	Ernest L. Hardin	6786
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