Features, Events and Processes and Performance Assessment Scenarios for Alternative Dual-Purpose Canister Disposal Concepts

Fuel Cycle Research & Development

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Ernest Hardin and Charles Bryan Sandia National Laboratories Michael Voegele Complex Systems Group, LLC

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FEATURES, EVENTS AND PROCESSES AND PERFORMANCE ASSESSMENT SCENARIOS FOR ALTERNATIVE DUAL-PURPOSE CANISTER DISPOSAL CONCEPTS

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> Ernest Hardin and Charles Bryan Sandia National Laboratories

ABSTRACT

Options for disposal of commercial spent nuclear fuel could be expanded by demonstrating the safety and feasibility of directly disposing of fuel that has been stored in existing dual-purpose (storage and transportation) canisters. The safety aspects will be addressed using performance assessment, a probabilistic risk analysis methodology that has been applied to geologic disposal in the U.S. and other countries. The methodology relies on systematic identification of features, events and processes that could be significant to performance and should be included in the assessment. For the dual-purpose canister disposal application, this report identifies key features, events and processes that can distinguish direct disposal of fuel in existing dual-purpose canisters from disposal of the same fuel in smaller canisters designed specifically for disposal. It also identifies which scenarios should be considered, including nominal and human intrusion, and what numerical schemes are available and appropriate to conduct performance assessments with the expected level of detail.

Introduction

The purpose of performance assessment (PA) in evaluating the feasibility of direct disposal of spent nuclear fuel (SNF) in dual-purpose canisters (DPCs), such as those that currently exist, is to generate recommendations as to whether disposal can be accomplished safely as defined by regulatory performance objectives. The assessments will model the implementation of safety strategies developed by Pierce et al. (2013), for selected DPC disposal concepts proposed by Hardin and Voegele (2013). The PAs will evaluate significant differences, if any, in postclosure waste isolation performance for DPC direct disposal, compared with repackaging the same SNF in purpose-built containers and disposal in the same geologic setting. The hypothetical purposebuilt containers could have any capacity, but would likely contain fewer SNF assemblies than DPCs.

The PAs will be generic, i.e., not site-specific, consistent with the current objectives of the Used Fuel Disposition (UFD) R&D program. This is reflected in the safety strategies, which identify and describe the functions for the engineered and natural barriers, for a total of six generic disposal concepts (Pierce et al. 2013). More concepts and variations are certainly possible, but these six (simplified to three below) are sufficient to support the safety aspects of feasibility evaluation.

This report recommends which FEPs from a comprehensive generic list (Freeze et al. 2011) should be included in a base case, and which might be included in more detailed assessments with greater detail ("simulation case" assessments). The base case is described here with a minimum number of included FEPs to facilitate model development. This report also includes a discussion of possible additional simulation cases that could be used to represent and evaluate certain FEPs with greater detail.

In general, PA models are developed for defined cases which are then grouped into scenarios or scenario classes. Scenario classes are based on separate and independent initiating conditions or events (e.g., separate nominal scenario, human intrusion scenario, etc.) so that the probabilityweighted consequences for scenario each can be summed (or convolved using annual event probabilities) to assess system performance. This report recommends scenario classes for structuring assessments of DPC direct disposal safety. Finally, it briefly discusses software tools and numerical strategies that could be sufficient for implementing first a base case model, then more detailed simulation cases. Importantly, for any tool selected the PAs will be supported by side calculations, abstractions, uncertainty estimates, and other inputs.

1. Disposal Concepts for Performance Assessment

A disposal concept is defined to consist of a waste stream, geologic setting, and engineering concept of operations. Alternative concepts for disposal of commercial SNF in various settings using appropriate concepts of operation, were proposed by Hardin and Voegele (2013) based on earlier work (Hardin et al. 2012). These were reviewed by Pierce et al. (2013) who selected six representative concepts for consideration of safety strategies and performance assessment:

- **Salt** An enclosed emplacement mode in bedded or domal salt, whereby waste packages would be emplaced on the floor and immediately covered with crushed salt backfill. A variation would emplace packages into large-diameter, vertical or horizontal boreholes constructed from underground disposal rooms or drifts. Fuel canisters would be sealed into disposal overpacks made from low-alloy steel. The host salt formation would gradually collapse onto the emplacement drifts, and the applied stress would reconsolidate the crushed salt backfill, fully encapsulating each package in salt with low porosity and very low permeability.
- **Hard-Rock Unbackfilled Open** A repository constructed in competent rock (e.g., igneous, metamorphic or well indurated carbonate or other sedimentary rock) using indrift emplacement, and forced ventilation for 50 to 100 years after waste emplacement. Emplacement drifts would remain open after closure (until eventual collapse). Because this concept does not use backfill or otherwise seal the emplacement rooms or drifts, its application is limited to unsaturated hydrogeologic settings. Disposal overpacks would be made from corrosion resistant materials for containment longevity in oxidizing disposal environments. Other engineered barriers (e.g., barrier coatings, drip shields, etc.) would be added as necessary for multiple-barrier defense-in-depth. This concept would be similar to that previously developed in the United States for this type of geologic setting (DOE 2008).
- **Hard Rock Backfilled Open** For application in saturated hydrogeologic settings the repository emplacement drifts, access drifts, and other openings would be ventilated for 50 to 100 years, then backfilled with low-permeability materials at closure to prevent preferential groundwater flow. Backfill would also control rock deformation (i.e., rockfall

and drift collapse) and limit the dynamic response to seismic ground motion. Swelling clay-based materials have been proposed to ensure low-permeability given practical limitations on the consistency of backfill emplacement (which are compensated by swelling behavior). However, clay-based materials may be sensitive to elevated temperature (e.g., above 100° C), limiting thermal loading at closure and thereby extending the required duration of surface decay storage and/or repository ventilation operations (Hardin and Voegele 2013).

- **Sedimentary Unbackfilled Open** In-drift disposal concept, designed to remain open and ventilated until the SNF age is 150 years out-of-reactor. Ground support would be designed to maintain opening stability sufficient for ventilation, and to control desiccation. At repository closure plugs and seals (but not backfill) would be installed to isolate waste packages, preventing preferential groundwater flow. Sedimentary settings would be selected for thickness and extent, low permeability, chemically reducing conditions, and tectonic stability. Peak temperature of the host rock would be limited (e.g., 100° C) to control thermal degradation. Accordingly, for hotter conditions (e.g., higher fuel burnup, less heat dissipation) longer decay storage and/or repository ventilation could be required.
- **Sedimentary Backfilled Open** Backfill could be added as an option any time during repository operations, right up to the time of closure. All waste emplacement and other openings would be backfilled. A structural backfill (e.g., sand or gravel) could be used in conjunction with the plugs and seals discussed above, to stabilize drift collapse behavior and limit dynamic response to seismic ground motion. Backfill with low permeability would also isolate packages and reduce the need for plugs and seals. Given the thermal limitations on the unbackfilled mode above, addition of backfill might impose only minor changes in the manner and timing of disposal.
- **Cavern-Retrievable** Storage and disposal facility developed within a few hundred meters of the ground surface, in competent rock capable of supporting large excavations (e.g., 8-m spans). Shielded, dry-cask storage systems such as those currently used for surface storage would be moved underground in the cavern, accessed by a waste handling ramp. After sufficient ventilation duration, or when the SNF age is 150 years out-ofreactor, the repository would be closed by fully encapsulating each cask with lowpermeability buffer/backfill material. Each cask would be self-shielding, facilitating access to the storage/disposal cavern for maintenance, moving or retrieval of casks, and closure operations.

With the exception of the salt concept, these selected disposal concepts are open emplacement modes whereby SNF waste packages would be emplaced in open drifts and ventilated for decades to remove heat. The enclosed modes described by Hardin et al. (2012) are based on disposal concepts being studied internationally, and they involve emplacing waste packages in direct contact with buffer, backfill, liner or host rock materials. For DPC direct disposal the enclosed modes would require decay storage (or repository ventilation) of many centuries, because of higher waste package heat output. The heat dissipation properties of salt, and its tolerance for temperatures of 200° C or higher, allow emplacement and immediate backfilling of large waste packages (e.g., 32-PWR or larger) after a few decades of decay storage (Hardin and Voegele 2013).

As a simplification, backfill can be represented by the base case, and the unbackfilled cases (hard rock and sedimentary, above) can be considered when additional FEPs (e.g., rockfall, drift collapse, mechanical damage, etc.) are included in "simulation case" assessments. As a further simplification, the cavern retrievable concept can be represented by the hard rock backfilled concept. The remaining three concepts are recommended for evaluation using a base case model:

- Salt Concept
- Hard Rock Backfilled Open Concept
- Sedimentary Backfilled Open Concept

The FEPs that would be included and excluded, and the PA scenarios that would be considered in the base case model are described in the following sections. For the other concepts discussed above in this section more process-level detail would be needed, for example to represent the effects from seismic ground motion for concepts that remain open after closure. The simulation cases described in Section 3.2 would include such additional detail.

2. Previous FEP Scoping Studies

A compact, generic set of FEPs was developed from international sources and prior experience in the U.S. (Freeze et al. 2011) and is currently being used by the UFD Campaign in the disposal R&D program. The FEP list was analyzed by Vaughn et al. (2011) who identified FEPs that were included in generic performance assessments for repositories in clay/shale media, crystalline rock, salt, and the deep crystalline basement (deep borehole disposal concept). The results for these three generic mined-disposal PA models are summarized in Table 1 of this report. The 2011 study included a generic PA model for clay/shale media that is considered below for use as the base case for DPC direct disposal PA.

Among the generic FEPs, some were identified in a planning exercise ("R&D Roadmap") as warranting more investigation because of the state of knowledge and the potential impact on waste isolation performance (Nutt 2011). Among these high priority FEPs the ones likely to distinguish DPC direct disposal from other disposal concepts are shown in Table 1.

A later analysis of FEPs considered which should be included in the engineered barrier system (EBS) components of a next-generation PA (Hardin 2012). The list identifies a simpler case that could be readily implemented, and a more advanced case that could be used to evaluate impacts from additional processes and repository design features. The FEP list for the simpler case is included in Table 1 and compared to that recommended here for DPC PA.

3. Features, Events and Processes

This section identifies a minimum set of FEPs that could be included in a base case for evaluating DPC disposal safety. FEPs recommended for inclusion in a base case and more detailed "simulation" cases are listed in Table 1. Given the extent of previous FEP studies, there is little need to reiterate except to point out which FEPs are needed to distinguish DPC direct disposal from repackaging and disposal of the same SNF in purpose-built disposal canisters.

The base case and simulation cases reference a disposal system architecture (Figure 1). This depiction is adapted to both advection and diffusion dominated transport environments, and includes advective conditions upstream as well as downstream.

Upstream (Flow) Upstream (Flow) Downstream (F&T)																									
		Natural System												Engineered Barrier system (EBS)							Natural System			Receptor	
Recharge	Aquifer	Host Rock	EDZ	EBS -Field ത	Near-Field EBS	features) diversion ş	Eorn Waste	Insert	Filler	(structural ŝ	ã containm features) ŝ	features)	Support $\hat{\mathsf{s}}$	Buffer Clay	Envelope	은 $\overline{\mathbf{a}}$ œ π Bal	ਫ਼	<u>ត្រ</u>	etc.) (other plugs, EBS seals Far-Field WP _S	EDZ	Host Rock	Aquifer	ಿಕ Atmospheric July Surface	Biosphere	
Notes:																									
1. Clay Buffer = Includes reservoir used to manage heat and/or multiphase flow around waste packages																									
					2. Envelope = container for pre-fab. EBS																				

Figure 1. Disposal System Architecture (from Hardin 2012)

Potential differences between direct disposal of DPCs and disposal of the same SNF in packages (including canisters) designed for disposal, may include:

- **Emplacement Mode and EBS Design –** With the exception of the salt disposal concept, DPC disposal concepts are open emplacement modes that use ventilation to remove heat. Whereas the enclosed modes in crystalline and sedimentary rock types (Hardin et al. 2012) have low-permeability, clay-based swelling buffer materials directly contacting the waste package; the open modes differ with respect to materials present in the near field. For the open modes waste packages may be surrounded by void space, or by backfill installed at closure. After closure, void spaces will gradually fill with debris from rockfall and collapse. Backfill emplaced remotely in emplacement drifts will have less density and uniformity than manually emplaced buffer/backfill materials. Hence, comparisons of DPC direct disposal with other concepts involving repackaging, are likely to include effects associated with greater permeability and potential for radionuclide transport in the near field.
- **Thermal Effects (comparing DPC direct disposal to other open modes)** The most common DPC sizes currently in use have the capacity for 24- or 32-PWR assemblies (or BWR equivalent). Future DPCs may contain more SNF, such as the Magnastor 37-PWR canister recently developed by NAC International. DPCs are not necessarily much larger than purpose-built disposal canisters, depending on the disposal concept under consideration. For example, previously in the United States the transport/aging/disposal (TAD) canister was designed to contain 21 pressurized water reactor (PWR) assemblies. A 21-PWR reference package size was recommended for open emplacement modes (Hardin et al. 2012). In both applications the 21-PWR size reduces the number of packages required to dispose of the U.S. SNF inventory, compared to smaller packages used with enclosed modes, while taking advantage of thermal management by the extended ventilation that is possible with open modes.

Peak temperatures for larger-capacity packages can be controlled by decay storage and repository ventilation, but post-peak temperature will remain higher for hundreds to thousands of years. (Aging can attenuate short-lived fission products, but larger packages contain more heat-generating actinides with intermediate half-lives, such as 241 Am.)

Thus, although the peak drift wall temperature can be managed and may be equivalent for 21 and 32 PWR sizes, for larger packages containing more SNF the peak temperature further into the host rock may be greater, and elevated temperature is likely to persist longer. In the backfill, the extent and duration of elevated temperatures (e.g., in the axial direction between packages) will also be greater. These differences can eventually impact radionuclide transport if the controlling rock and backfill characteristics are thermally sensitive. The direction of affected radionuclide transport could be radial or axial.

 Thermal Effects (comparing DPC direct disposal to enclosed modes) – Enclosed emplacement modes in crystalline and sedimentary rock types were shown to require 4- PWR size waste packages (or smaller) to limit peak temperature at the waste package surface to less than 100° C (Hardin et al. 2012). The additional time required for 50-year old SNF to cool by 8-fold (the difference between 32 and four assemblies per package) is on the order of 400 to 1,000 years depending on burnup. It is impractical to cool DPCs that long before disposal (see assumptions from Miller et al. 2012) and even after disposal they would have greater heat output than smaller canisters as discussed above. Thus, both the peak temperature throughout the near field, and the duration of elevated temperature, will generally be greater for in-drift disposal of DPC-based packages (with decades of repository ventilation) than for smaller packages using enclosed emplacement modes (without extended ventilation). Thermal effects from DPC direct disposal could be radial or axial as discussed above, while performance of enclosed modes would more closely resemble that analyzed for the Swedish (SKB 2011) and French (Andra 2005) SNF disposal concepts. In accordance with this discussion, assessment of DPC direct disposal should include thermal effects on the near-field environment, especially when compared with alternative enclosed modes of SNF disposal in much smaller packages.

A notable exception to the need for small packages with enclosed emplacement modes is the salt repository concept, which can accommodate SNF waste packages up to 32-PWR size or larger (or BWR equivalent). Peak salt temperature is directly related to package thermal power at emplacement, and the power limit can be met by 32-PWR size packages with high-burnup SNF, after decay storage of approximately 70 years (Hardin and Voegele 2013). A reference 12-PWR package size was selected previously based on shaft hoist considerations (Hardin et al. 2012).

- **Quantity of SNF –** Once a waste package breach occurs more SNF will be exposed to the disposal environment with DPCs, than with smaller containers. The difference would be greatest in comparing DPCs with smaller canisters (4-PWR size) used for enclosed emplacement modes. The greatest potential for differences in radionuclide mobility would result from advection dominated transport, which is not expected for disposal concepts in low-permeability host media (except possibly for human intrusion scenarios) but might occur. Even the most massive, homogeneous sedimentary host units can be traversed by through-going discontinuities with greater permeability, such as faults or fracture zones which could act as advective pathways in and out of the emplacement drifts. The possibility for advection dominated transport is a factor of interest in the safety of DPC direct disposal, related to quantity of SNF per package.
- **Inner Canister Design** Canisters purpose-built for disposal may have different features not found in existing DPCs, such as: inserts (in lieu of baskets); thicker shells, plates

and/or spacers to extend structural lifetime in corrosion environments; thicker neutron absorbing elements that can function after $10⁴$ years of degradation; and fillers that can exclude moderating groundwater after package breach. Existing DPCs cannot include any of these features (assuming they cannot be reopened) which is the major reason that the potential for postclosure criticality may be greater for some disposal concepts.

For comparison of DPC direct disposal with disposal of the same waste repackaged in purposedesigned containers using the same *open* emplacement mode, performance of the SNF waste form, waste package, other engineered barriers, and the far field will be simliar (i.e., same concept and safety strategy). Relating to package size, thermal effects and inner canister design are potentially important. Impacts from inner canister design differences may be limited to the technical analysis that is relied upon to disposition postclosure criticality (FEP 2.1.14.01, see Table 1). Quantity of SNF is likely not significant for comparing packages differing only slightly in size (e.g., 21- vs. 32-PWR) but will be more important for comparing to alternative concepts involving much smaller packages (discussed below). In accordance with this discussion, the FEPs needed for comparing DPC direct disposal with similar *open* modes of emplacement are limited to an appropriate base case that includes thermal effects and advective transport of radionuclides (as well as other transport processes).

For comparing DPC disposal to disposal of the same SNF in the same host medium but smaller canisters using an *enclosed* emplacement mode, more FEPs need to be included. For example, reference enclosed crystalline or clay/shale concepts for spent fuel use 4-PWR packages encapsulated in clay-based swelling buffer/backfill, which would involve buffer degradation (FEP 2.1.04.01). The additional FEPs needed to compare *open* emplacement of DPC-based packages (with backfilling at closure) vs. *enclosed* emplacement of smaller waste packages, are included among those recommended for the base case (Table 1).

All canisters, whether existing DPCs or purpose-built for disposal, will have disposal overpacks (Hardin et al. 2012; Hardin and Voegele 2013). These will provide additional benefits to the safety of handling, transport and emplacement in the repository, and provide containment integrity for some period of time after emplacement. Disposal overpacks for existing DPCs might differ with respect to dimensions, shape and lifting features. However, for this study they can be assumed to have the same characteristics as disposal overpacks for purpose-built disposal canisters, such as material type, thickness, fabrication method, surface treatment, etc., that could affect waste isolation performance.

The value of generic assessments is increased when the assessments include comparisons to cases in which DPCs are repackaged, and the same SNF is emplaced in purpose-built waste packages in the same geologic setting.

3.1 Base Case

The base case is designed to be implemented using off-the-shelf system modeling software. As discussed in Section 5, a standardized model framework can be used, and the connectivity of model components and the uncertainty distributions describing key parameters can be modified to represent different disposal concepts. A base case model implemented this way will have limited dimensionality (e.g., 1-D or 2-D) and will rely on simplifications or abstractions, especially to represent processes in the near-field and EBS (Vaughn et al. 2011).

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FEPs applicable to the base case model for DPC disposal (and for alternative concepts with smaller, purpose-built canisters) are listed in Table 1. Formulation of the base case is predicated on the following model limitations and FEP exclusion rationale:

- Preclosure events and processes do not affect postclosure performance and/or do not discriminate direct disposal of DPCs (Table 1, Section 1.1.00.00).
- Seismic and faulting events do not significantly impact the natural system and biosphere, which have been exposed to these events for geologic time (FEPs 1.2.03.02, 1.2.03.03 and 2.2.05.03).
- Mechanical degradation and seismic ground motion do not significantly affect backfilled underground systems (include FEP 2.1.07.03; exclude FEP 1.2.03.01; Table 1, Section 2.1.07.00; and FEP 2.1.11.04).
- Faulting does not affect the repository (potential slip on unrecognized faults is minor) (FEP 2.1.07.10).
- Igneous activity has very low probability of disrupting the repository (Table 1, Section 1.2.04.00).
- Other, long-term processes (tectonophysics, dissolution, astronomical) can be excluded (Table 1, Sections 1.2.01.00 and 1.5.00.00).
- Climate change (natural or anthropogenic; Table 1, Section 1.3.00.00) can be addressed in the base-case model by changing groundwater flow boundary conditions (FEP 2.2.08.03).
- Future human actions are limited to inadvertent human intrusion (Table 1, Section 1.4.00.00).
- Heterogeneity and co-location of the waste inventory (FEPs 2.1.01.03 and 2.1.01.04) can be addressed in the base case model by considering a range of age and burnup for commercial SNF without considering location in a repository.
- Cladding will be conservatively neglected in the base case (FEP 2.1.02.06) although partial credit for cladding containment may be taken in a more complete simulation case.
- Early waste package failure and modes of waste package corrosion are potentially significant for corrosion-resistant disposal overpacks, but much less so for corrosion allowance materials intended to have shorter corrosion lifetimes (FEPs 2.1.03.01 through 2.1.03.07).
- Evolution of flow pathways within failed packages can be neglected using a simplification that flow occurs within failed packages without restriction (FEP 2.1.03.08).
- Backfill is not degraded by mechanical or chemical processes (FEPs 2.1.04.01 and 2.1.07.04) although clay-based backfill and buffer materials may be eroded by groundwater flow (FEP 2.1.04.01).
- Radionuclide mobility is not affected by mechanical loading of waste forms, loading at interfaces, or other mechanical degradation processes in the EBS.
- Flow in the EBS can be represented using simplified approaches, accounting for possible changes (FEP 2.1.08.06), but unsaturated flow (FEPs 2.1.08.07 through 2.1.08.09) and flow through far-field plugs and seals (FEPs 2.1.05.01 and 2.1.08.04) require more detailed models (see simulation cases described in Section 3.2).
- Chemical processes in the EBS can affect the rates of waste package and waste form degradation, and radionuclide transport. Base case model simplification is recommended using bounding approximations to those rates, supported by sensitivity analyses (FEPs 2.1.09.01 through 2.1.09.12; FEP 2.1.11.14).
- Colloids do not contribute significantly to radionuclide transport because of limited mobility in low-permeability engineered and/or natural media (FEPs 2.1.09.55 through 2.1.09.61; FEPs 2.2.09.59 and 2.2.09.60).
- Thermal effects on flow and transport can be neglected (FEPs 2.1.11.02, 2.1.11.04, 2.1.11.05, and 2.1.11.08 through 2.1.11.13) as relatively brief transients that occur before most radionuclide releases. A minor exception is elevated waste package temperature from insulation by backfill, which may affect degradation of the disposal overpack, but can be readily evaluated in the base case using simple models.
- Disposal overpacks are resistant to thermally driven degradation, or provide corrosion allowance (FEP 2.1.11.07).
- Seals and plugs are located outside the influence of heating (FEP 2.1.11.09).
- Gas generation from corrosion of steels is a second-order influence on radionuclide mobility and transport for the base case (Table 1, Section 2.1.12.00).
- Radiation effects in the disposal environment (e.g., radiolysis, radiation damage) can be taken into account by adjusting degradation rates and solubilities (Table 1, Section 2.1.13.00).
- For the base case, in-package nuclear criticality (Table 1, Section 2.1.14.00) may be excluded based on insufficient water accumulation to flood breached waste packages (FEP 2.1.08.02) and/or the presence of neutron absorbers (e.g., borate or chloride) in the influent water (FEP 2.1.09.02).
- Criticality in the EBS or near field (FEP 2.1.14.02) is very unlikely because of homogeneous hydrochemical conditions that promote dissipation rather than concentration of fissile radionuclides, and/or moderator exclusion and the presence of neutron absorbers.
- Far-field flow and transport in the host rock formation and other units are substantially unchanged by repository excavation, mechanical effects, unsaturated flow processes, dehydration, surface water discharge, and thermally driven processes (FEP 2.2.05.03; Table 1, Section 2.2.07.00; FEPs 2.2.08.04 and 2.2.08.05; FEPs 2.2.08.07 and 2.2.08.08).
- Chemical processes in the far field can be neglected (or do not discriminate direct disposal of DPCs) if simplified bounding approaches to radionuclide transport are used (FEPs 2.2.09.01 through 2.2.09.04; FEPs 2.2.09.57 and FEPs 2.2.09.58).
- Isotope dilution of ^{129}I by stable ^{127}I in the geosphere does not affect dose calculations, i.e., the total iodide concentration is so small that all iodide ingested is absorbed (FEP 2.2.09.63).
- Biological processes do not significantly affect radionuclide transport in the far field (Table 1, Section 2.2.10.00).
- Thermal processes, gas generation, and nuclear criticality are not significant in the far field (Table 1, Sections 2.2.11.00, 2.2.12.00 and 2.2.14.00).
- Surface characteristics and surficial mechanical, hydrologic, chemical, biological and thermal processes do not discriminate direct disposal of DPCs (Table 1, Section 2.3.00.00).
- Human behavior and biosphere characteristics do not discriminate direct disposal of DPCs (Table 1, Sections 2.4.00.00 and 3.0.00.00).

The base case described here and in Table 1 is intended to represent the three disposal concepts identifed in Section 1:

- Salt Concept
- Hard Rock Backfilled Open Concept
- Sedimentary Backfilled Open Concept

with the following features in common: 1) corrosion allowance waste packaging (e.g., low-alloy steel); 2) saturated, low-permeability host medium; 3) emplacement drift backfill; 4) disturbed rock zone (DRZ) development; 5) advective and diffusive transport of radionuclides; 6) insignificant colloid and biocolloidal radionuclide mobility; and 7) no significant effects on radionuclide mobility from thermally driven processes or repository introduced materials. Various FEPs such as those representing multi-phase thermally driven processes, corrosionresistant packaging, and consequences from seismic ground motion, may be added to represent the other concepts discussed in Section 1.

The base case approach will represent various FEPs using abstracted component models with input parameter settings based on judgment, supporting analyses, and/or analyses from previous studies. Processes to be represented this way in the nominal scenario include waste package and waste form degradation, solubility controls, sorption, and radionuclide transport (head gradient, conductivity, diffusion or flow area, path length).

3.2 Simulation Cases

The simulation cases described here identify the types of models that could provide addtional process-level detail for DPC PA. Additional FEPs that could be included for this purpose are listed in Table 1. The additional detail could be abstracted to augment the base case model, or an entirely different approach could be used. For example, integrated disposal system performance could be represented by merging component models with a "host" multi-physics simulator (Hardin 2012).

Lumped Parameter Model for Near-Field Chemistry – A "mixing cell" approach for modeling water chemistry in the near-field EBS is appropriate for non-advecting or slowly advecting conditions. This simulation case would be used to investigate the relationship between quantity of SNF (Section 3) and advective transport conditions. The composition of influx may be represented by formation waters (FEPs 2.1.08.01 and 2.1.09.01). Near-field waters interact with engineered materials, corrosion products, the waste form, and released radionuclides (FEPs 2.1.09.05 through 2.1.09.10, and 2.1.09.53). The near-field EBS water composition (FEPs 2.1.09.02 through 2.1.09.04) serves as a concentration boundary condition for diffusive transport (FEP 2.1.09.52) and as the composition of advective outflux (FEP 2.1.09.51), for example, associated with human intrusion.

Backfill Options – This simulation case could be used to quantify the relationship between quantity of SNF (Section 3) and radionuclide transport, for alternative backfill materials and schemes for plugging and sealing (FEPs 2.1.08.01, 2.1.08.02, 2.1.08.03 and 2.1.08.06). Functions assigned to backfill may include isolating waste packages by limiting radionuclide diffusive and advective transport, and stabilizing openings in the host rock. Low-permeability mixtures of swelling clay with sand or crushed rock have been studied extensively (SKB 2010), but emplacing such materials remotely, in a radiological environment, as would be necessary for some DPC direct disposal concepts, presents technical challenges for implementation and verification (Hardin and Voegele 2013). If the backfill function is limited to stabilizing openings (limiting further development of the DRZ after closure) then other materials, such as sand or non-swelling clay, could be used in conjunction with plugs and seals that compartmentalize emplacement areas. However, a more permeable backfill could promote advective transport, particularly in the human intrusion scenario (Section 4).

Thermally Driven Coupled Processes – The hotter conditions of DPC direct disposal could be important if thermally driven processes cause long-duration changes in the EBS or host medium. Changes such as fracture or matrix porosity changes, dewatering, bulk rock shrinkage, mineral alteration, reduction of surface area, etc., could affect flow into and within the EBS (FEPs 2.1.11.10 and 2.1.11.11). Numerical simulation of coupled chemical processes in the host rock and backfill can produce localized alteration of conditions affecting EBS performance and radionuclide transport (FEPs 2.1.04.01, 2.1.08.06, 2.1.08.09, 2.1.09.01, 2.1.09.03, 2.1.09.06 and 2.1.11.13). Beyond the influence of repository heating, for example in the far field where plugs and seals are installed, this simulation case would not discriminate direct disposal of DPCs.

Waste Package Degradation Mechanisms and Partial Containment – Containment lifetime is an objective for disposal concepts that protect SNF from the disposal environment for $10⁴$ years or longer to lower the probability of certain FEPs (e.g., postclosure criticality FEP 2.1.14.01). For example, containment is a key function of the waste package for the hard rock unsaturated concept, and corrosion-resistant materials would be used (Pierce et al. 2013). Corrosion-resistant disposal overpacks are also identified as an option for other DPC disposal concepts depending on site-specific and/or regulatory factors. Containment integrity for these concepts may be impacted by several processes such as general corrosion, stress corrosion cracking, localized corrosion, and microbially influenced corrosion (FEPs 2.1.03.02 through 2.1.03.05). These processes depend on temperature and other environmental conditions, and thus, may discriminate direct disposal of DPCs.

A simple model enhancement could represent total containment followed by time-dependent breach (instead of a fixed containment lifetime) caused by a single, dominant corrosion mechanism. A more complex simulation case could include multiple corrosion mechanisms, accounting for spatially variable corrosion over the surface of each package, and gradual degradation after initial breach. Also, it could account for restriction of water movement within or through degraded packages (FEP 2.1.08.02).

Seismic Ground Motion and Drift Collapse – For the unbackfilled DPC direct disposal concepts (Section 1) rockfall and drift collapse will eventually degrade the emplacement openings, potentially impacting engineered barriers such as the waste package (FEPs 2.1.07.01, 2.1.07.02, 2.1.07.05 and 2.1.07.06). Seismic initiation will increase the frequency of rockfall and drift collapse, depending on the seismic hazard (FEP 1.2.03.01), so static and seismically induced drift degradation should be modeled together. In particular, where waste package containment lifetime is an important part of the performance strategy with unbackfilled emplacement drifts, rockfall and drift collapse are potentially important to waste isolation performance (e.g., DOE 2008, Section 2.3.4).

Modeling approaches similar to those used in the past for the hard-rock unsaturated concept (e.g., distinct element; SNL 2004) can be used for static and dynamic (seismic initiation) analysis. Extensive seismic response calculations were performed for the Yucca Mountain license application (SNL 2007). These showed that: 1) corrosion resistant waste packages in open drifts can accumulate damage (e.g., residual stress); and 2) waste packages surrounded by fill (e.g., rockfall debris, or engineered buffer or backfill) sustain little or no damage from seismic ground motion. Dynamic calculations generally have not included in-package structural response (FEPs 1.2.03.01 and 2.1.07.10). In open drifts the potential for dynamic damage to cladding leads to an assumption that all cladding is breached, while for concepts that have corrosion-allowance overpacks in backfilled drifts the physical condition of the overpack, canister, basket, and fuel cladding is highly uncertain after degradation.

Unsaturated Flow in the Host Rock – For comparison of DPC disposal with alternative concepts in the unsaturated zone, multi-phase flow and thermally driven flow processes are potentially important. The controlling FEPs are the same as for saturated flow (e.g., FEPs 2.1.08.1, 2.1.08.02, 2.2.08.01 and 2.2.08.02) but the conceptual, mathematical and numerical models are different. Simulation can be accomplished using existing thermal-hydrology process models, coupled as necessary with chemical and mechanical processes.

Degradation of Far-Field Plugs and Seals – Degradation of far-field engineered barriers could change groundwater flow patterns and facilitate advective transport of radionuclides through or along repository openings (FEPs 2.1.05.01 and 2.1.08.04). Although these far-field components are not (by location) affected by heat, their performance may be important in relation to the Quantity of SNF issue (Section 2) if there is significant advective transport of radionuclides. Simulation of plug and seal performance can be accomplished using groundwater flow codes taking into account flow contributions from backfill, the DRZ, undisturbed host rock, and other flow features that may be active.

4. Scenarios

The overall assessment of risk may combine probabilistically independent scenarios by summing the consequences calculated for each. As independent scenarios they depend only on the initial state of the system (common to all scenarios) and the class of events or event sequences that is unique to the scenario. In principle one event class could modify the nominal state of the system prior to an initiating event of a different class. However, the probability of each independent disruptive scenario is low enough that conjoint events need not be considered.

The nominal scenario is the starting point for building a total system performance assessment. It describes projected performance without disruptive events, and is required to include features and processes (except for disruptive events) that can significantly contribute to system performance. The possibility that one or more waste packages could be defective leads to the early failure component of the nominal scenario (FEP 2.1.03.01). There are many different ways that defects could arise, and predicting many of them is problematic, so an early failure component may be added based on a conservative, probability weighted consequence.

Human intrusion is a required part of the performance assessment, using a separate, stylized scenario to represent the dose consequence from future drillers inadvertently intersecting one or more waste packages and exposing the contents to transport by groundwater (e.g., 40CFR191 App. C). The stylized scenario is defined by regulation, independently from other scenarios including seismic ground motion and postclosure criticality. The potential for changes in the probability of human intrusion associated with direct disposal of DPCs, is evaluated in Appendix A for repositories for SNF, using large waste packages such as would be used for DPC direct disposal, in salt and hard rock geologic settings. The results indicate that the expected number of intersections is greater than 1, particularly for the salt case (and other sedimentary settings by analogy), and for horizontal waste package orientation.

Previous studies (Pratt et al. 1979; SNL 2007) have shown that seismic ground motion has no significant effect on backfilled underground facilities. Also, faulting of the host rock has been excluded or limited in previous performance assessments (SNL 2008; SKB 2011). For a backfilled repository that is situated where there are limited seismic and fault displacement hazards, it is reasonable to anticipate that seismic ground motion and its consequences (FEPs 1.2.03.01, and 2.1.07.01 through 2.1.07.04) could be excluded from PA so that no seismic scenario would be needed. For an unbackfilled repository subject to seismic hazard of sufficient likelihood, a mechanistic representation of ground motion effects would be needed to support a seismic consequence model.

Postclosure criticality is treated as a separate scenario that can be formulated, for example, based on an event tree approach (Rechard et al. 1996). Since the probability of volcanic disruption of the repository is assumed for the present study to be less than 10^{-8} per year, seismicity is the only other disruptive event that might have a high enough joint probability with a criticality event, for the combination to be included in PA. However, seismic FEPs can be excluded for backfilled repositories (see above; FEPs 1.2.03.01 and 2.1.07.01, so its consequences are limited, and criticality can likely be considered in a separate scenario from seismic events (if neither moderator exclusion or groundwater salinity is effective as discussed in Section 3.1).

5. Numerical Implementation

In a previous study Wang et al. (2011) assessed the state of the art in numerical simulation of coupled processes, including numerical simulation codes. They identified a dichotomy between simple PA models and process-level models that incorporate coupled physics and numerical simulation grids. The base case model described in this report is such a simple PA model, that can be implemented using off-the-shelf modeling software. The "simulation cases" would use process-level models adapted as input to PA, to capture coupled processes.

A set of simple PA models was developed by Vaughn et al. (2011) for repositories in clay/shale media, salt, crystalline rock and deep boreholes. In particular, the clay/shale model is structured and versatile, and runs entirely within the GoldSim® software application (a trademark of GoldSim Technology Group). This software was developed to represent systems with both engineered and natural components, incorporating uncertainty and applying Monte Carlo methods. It is the result of extensive development activities, which for many years were driven by the Yucca Mountain repository project.

The clay/shale model from Vaughn et al. (2011) includes "mixing cells" for waste form, waste package, a second engineered barrier, a DRZ, and the far field (Figure 2). Multiple cells are used to discretize these features, and the cells are connected by advective-diffusive pathways. Waste form and waste package degradation parameters (waste quantity and degradation rate, package lifetime, temperature dependence), groundwater flow parameters (flow area and path length, flux, velocity) and radionuclide transport parameters (representing diffusion and sorption) are input as uncertainty distributions. Parameters are used to tailor individual elements and the connectivity between them, to represent different disposal concepts. The 2-D far-field part of the model can be used to represent axial and radial variation of a DRZ (Figure 2). With appropriate development of inputs the approach is suitable for modeling the base case described in this report, especially with emphasis on comparisons between DPC direct disposal and alternative concepts involving repackaging.

The base case will use abstracted inputs such as uncertainty distributions for transport path lengths, velocities, and transport properties for radionuclides. It will use temperature histories from supporting calculations, as input to waste form and waste package degradation components, and to assign damage conditions to engineered barriers and the DRZ. It will use functions to represent waste package corrosion damage and waste form degradation. Most of these inputs will be developed separately for different concepts. The simulation cases discussed here can use the same GoldSim software, with additional effort applied to evaluating and abstracting inputs (e.g., the approach used for DOE 2008). To avoid too much complexity leading to loss of transparency, enhancements for each simulation case can be implemented in separate GoldSim input files.

A more advanced numerical model architecture was described previously (Hardin 2012) and is the ultimate goal of model development. It would replace the off-the-shelf modeling software, such as GoldSim, with a detailed numerical grid and multi-physics simulation algorithms that could include multi-phase nonisothermal flow and reactive chemical transport. The idea is to avoid abstractions to the extent possible, and to run all model components together simultaneously in a high-performance computing environment. In this approach the PA model would always use such a numerical "host" simulation for the natural system, although it might have limited dimensionality and could even be 1-D if that satisfies the application requirements. The EBS would be represented as a subdomain for each waste package within the host simulation, where multi-physics couplings are activated, specific to local processes such as corrosion of metallic components, evolution of EBS flow paths, sorption on corrosion products, etc. Uncertainty and successive realizations of the model would be managed at runtime using a shell such as DAKOTA (Freeze and Vaughn 2012).

NOTE: The "swept-away" boundary condition for Aquifer refers to the assumption of a very large volumetric flow rate in the aquifer (to a sink), which effectively removes any radionuclides released from the clay far field.

Figure 2. Schematic of Clay/Shale Model Far Field (Figure 3.3-9 from Vaughn et al. 2011)

6. Summary

Performance assessments will be used to evaluate the dose consequences of DPC direct disposal. The reduced set of disposal concepts for which representative DPC direct disposal will be evaluated consists of:

- Salt Concept
- Hard Rock Backfilled Open Concept
- Sedimentary Backfilled Open Concept

These concepts are further described elsewhere (Hardin and Voegele 2013). PAs will evaluate both the waste isolation performance of these three concepts for DPC direct disposal, and the differences in performance if the DPCs are repackaged, so that the same SNF is emplaced in purpose-built waste packages in the same geologic setting. A base case PA is proposed, and a set of simulation cases that would use increased model complexity and additional process-level simulations to address particular questions. Working with a previously described set of generic FEPs (Freeze et al. 2011), the FEPs that would be included in a base case, and a set of simulation cases, are identified (Table 1).

The recommended FEPs to be included are sufficient to address a set of topics representing potentially important differences between DPC direct disposal and disposal of the same SNF in purpose-built packages that are likely to be smaller. The topics identified in Section 3 are: emplacement mode and EBS design, thermal effects (comparing DPC direct disposal to other open modes), thermal effects (comparing to enclosed modes), quantity of SNF, and inner canister design.

The proposed base case would include: 1) corrosion allowance waste packaging (e.g., low-alloy steel); 2) saturated, low-permeability host medium; 3) emplacement drift backfill; 4) disturbed rock zone (DRZ) development; 5) advective and/or diffusive transport of radionuclides; 6) insignificant colloid and biocolloidal mobility; and 7) no significant effects on radionuclide mobility from thermally driven processes or repository introduced materials. The base case would represent backfilled openings and therefore does not need to consider rockfall, collapse, or effects from seismic ground motion.

More advanced simulation cases suggested in this report include additional model refinements to represent:

- Lumped parameter model for near-field chemistry
- Backfill options
- Thermally driven coupled processes
- Waste package degradation mechanisms and partial containment
- Consequences from seismic ground motion and drift collapse

These cases would require modeling capabilities such as integrated or abstracted geochemistry models, fully coupled multi-physics simulations, high-resolution waste package degradation and flow models, ground motion histories representing seismic hazard, and dynamic simulation of the effects of ground motion in open drifts and the surrounding rock.

A review of scenarios needed to implement total system PA shows that the base case representation of (backfilled) concepts would need: 1) nominal scenario; 2) human intrusion scenario; and 3) criticality scenario (unless postclosure criticality FEPs 2.1.14.01 and 2.1.14.02 are excluded).

Finally, a suggested approach for numerical implementation of the base case model is to use offthe-shelf software to model waste form and engineered barrier degradation and radionuclide transport, incorporating uncertainty and applying Monte Carlo methods to generate successive realizations of total system performance. The base case would use abstracted inputs such as temperature histories from supporting calculations, functions to represent waste package and waste form degradation, and uncertainty distributions for radionuclide transport parameters. Most of these inputs will be developed separately for different concepts. The simulation cases discussed here could either use the same off-the-shelf software, but with greater effort applied to evaluating and abstracting inputs, or the entire system could be represented in a numerical simulator.

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¹From Vaughn et al. (2011). Any FEP that is reported as partially included has "Note 1" inserted here. This generally includes FEPs that could be implemented by changing

parameter values based on judgment or other input, but which were not necessarily addressed in the Vaughn et al. (2011) generic PA models.
² FEPS identified as high priority by Nutt (2011), with potential to distinguish

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Appendix A –Human Intrusion Scenarios for Spent Nuclear Fuel: Borehole/Waste Package Intersections

A.1 Introduction

In many spent nuclear fuel (SNF) repository concepts currently under consideration, a major contribution to dose could be human intrusion via inadvertent drilling into the subsurface repository. Parameters for assessing human intrusion describe the number of holes drilled through the repository, and the number of waste packages intersected. For hard rock (represented by crystalline rock in this analysis) the likelihood of drilling through the repository is lower, as discussed below. In sedimentary host rock (e.g., salt or shale) a repository is more likely to be situated proximal to economic resources such as oil and gas, coal, or potash. Gasda et al. (2004) evaluated well densities in the Alberta Basin, and found more than 200,000 wells over an area of 468,000 km², yielding an average frequency of 0.48 wells/km². In a similar study, Nicot (2009) documented oil and gas wells in Texas and found over 1.1 million, mostly in the Permian Basin and along the Gulf Coast. In the Gulf Coast more than 125,000 wells were identified in an area of approximately 50,000 km^2 , yielding an average density of 2.4 wells/ km^2 . Note that with most oil and gas exploration and development the boreholes tend to be clustered, for example Nicot (2009) found local densities as high as 100 wells/ km^2 near salt domes. This uncertainty is part of the reason for using stylized scenarios with borehole frequency or waste package intersection rates specified by regulation.

Recognizing the variability and uncertainty in drilling rates, 40 CFR 191 (Appendix C) "*Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High Level and Transuranic Radioactive Wastes*" states that:

...the likelihood of such inadvertent and intermittent drilling need not be taken to be greater than 30 boreholes per square kilometer of repository area per 10,000 years for geologic repositories in proximity to sedimentary rock formations, or more than 3 boreholes per square kilometer per 10,000 years for repositories in other geologic formations.

While 40 CFR 191 provides general regulations for assessing the frequency of human intrusion, these are generally superseded by site-specific regulations. The only existing site-specific regulation for a SNF repository in the U.S. is 10 CFR 63: "*Disposal of High Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada*." The stylized scenario described in this regulation considers the impact of one borehole intersecting a waste package. By comparison, regulations for the Waste Isolation Pilot Plant (WIPP), a repository for transuranic waste (40 CFR 194: "*Criteria for the Certification and Re-Certification of the Waste Isolation Pilot Plant's Compliance with the 40 CFR Part 191 Disposal Regulations*") state that the frequency of boreholes drilled through the repository is more than 58 boreholes/ km^2 per 10,000 years (DOE 2009).

This appendix assesses the number of borehole-waste package intersections expected to occur for SNF repositories sited in hard rock settings and in sedimentary basins, based on the borehole frequency limits quoted above from 40 CFR 191: β boreholes/km² per 10,000 years for crystalline rock (representing hard rock options for this analysis), and 30 boreholes/km² per 10,000 years for sedimentary basins (e.g., salt or shale). It also examines how the number of borehole/waste package intersections varies with waste package size (ranging up to packages containing 32-PWR size DPCs or BWR equivalent) and orientation (horizontal or vertical).

Whereas the human intrusion assessment for the WIPP considers "cavings and cuttings" of waste that would be transferred to the surface by drilling (DOE 2009), the approach described in 10 CFR 63 ignores this potential dose pathway because it would not show "…how well a particular repository site and design would protect the public at large" (10CFR63, 66 FR 55732, p. 55761, Supplementary Information, 3.10 Human Intrusion Standard). The approaches to license application safety analysis described in 10 CFR 63 are assumed to be applicable to DPC direct disposal (Miller et al. 2012). However, 10 CFR 63 is specific to the Yucca Mountain site, so for this analysis the borehole frequency is assumed to be described by 40 CFR 191. For details of the Yucca Mountain and WIPP assessments the reader is referred to separately published analyses (SNL 2008; DOE 2009).

Regardless of how dose is calculated, any regulatory framework will require estimates of the number of borehole/waste package intersections. In low permeability host media radionuclide releases would likely be insignificant unless waste packages are actually penetrated. This appendix provides a framework for estimating the potential number of borehole/waste package intersections from drilling.

A.2 Parameters Needed

To calculate the potential number of borehole/waste package intersections for a repository, several parameters are needed:

Borehole frequency—As noted above, the rates from 40 CFR 191 are used. These are specified over a time frame of 10,000 years, which is the time limit for considering a human intrusion event, according to both 10 CFR 60 and 10 CFR63 (the consequences of human intrusion may be considered beyond 10,000 years).

Waste package dimensions—Package length and diameter are used to calculate cross-sectional area for horizontal and vertical emplacement (Table A-1). Several different package sizes are compared in order to assess the effects of waste package size and capacity on the number of fuel assemblies exposed by borehole/waste package intersections.

Source: Hardin et al. (2012, Tables 1.4-1 & 4-1)

Borehole diameter—It is assumed for this analysis that:

- Waste packages are substantially degraded when drilling occurs, so that any boreholewaste package intersection will expose the entire inventory of that waste package.
- Waste package degradation does not change the overall dimensions of the waste package.

These assumptions are generally consistent with previous analyses (e.g., DOE 2009) and they simplify the calculation. The borehole location can be treated as a single point in X-Y space, if the dimensions of the waste package "target" are increased by the radius of the borehole (Figure A-1).

Figure A-1. Schematic of Borehole–Waste Package Intersection Geometry

Borehole diameter is treated parametrically over a range from 8 to 13 inches. This range encompasses the 11-inch diameter typical of oil and gas boreholes that penetrate the Salado salt formation in southeastern New Mexico.

Repository layout—The layout determines the layout area per waste package, and the total repository area. This scoping analysis assumes that waste packages in sedimentary host media (and particularly salt) will be emplaced on a 30 m \times 30 m grid, or a single-package layout area of 900 m² per package. This area is appropriate for larger, hotter packages containing 32-PWR (or BWR equivalent) size DPCs (Hardin and Voegele 2013) and is greater than for previously described concepts with smaller packages (Hardin et al. 2012). For the hard rock repository, it is assumed that waste packages will be emplaced on a 20 m \times 70 m grid, corresponding to a singlepackage layout area of $1,400 \text{ m}^2$ per package (Hardin and Voegele 2013).

A.3 Calculating the Number of Intersections

A.3.1 Expected Number of Intersections

In the simplest approach, the mean probability of intersection per package, at any given borehole frequency (boreholes/km²), can be calculated from the cross-sectional plan area of a single waste package, regardless of the repository layout. It is given by the borehole frequency multiplied by the waste package cross-sectional area. Thus, for a sedimentary basin with a borehole frequency of 30 boreholes/ km^2 and a waste package cross-sectional area of 10 m²/package for each 32-PWR size package (Table A-1), the mean probability of intersection per package is 0.0003 $(= 10 \text{ m}^2 \times 10^{-6} \text{ km}^2/\text{m}^2 \times 30 \text{ boreholes/km}^2)$. Multiplying by the total number of waste packages in the repository (10,000 in this case) gives the expected number of borehole/waste package intersections per repository $(= 3 \text{ in this case}).$

Equivalently, the mean predicted number of intersections for the entire repository is equal to the total waste package cross-sectional area (km²) multiplied by the borehole frequency. For instance, in a 140,000 MT repository using 32-PWR size waste packages emplaced horizontally, the total waste package cross-sectional area is 0.1 km^2 (Table A-2). Thus, for an assumed sedimentary repository borehole frequency of 30 boreholes per km^2 , one would expect three waste package intersections per repository, accessing 96 SNF PWR assemblies.

The expected number of borehole/waste package intersections at a borehole frequency of 1 borehole/km² is equal to the total cross-sectional area of waste packages in a square kilometer, divided by 1 km². The expected number of intersections at any borehole frequency can be found by multiplying the frequency (in boreholes per km^2) by this result. Thus, the expected number of intersections varies linearly with the borehole frequency.

These results illustrate three points: 1) the expected number of intersections is much lower for waste packages emplaced vertically; 2) smaller packages have a greater total cross-sectional area and thus a greater expected probability of intersection than larger packages; and 3) although the expected probability of intersection is lower for larger packages, the expected number of exposed fuel assemblies *increases*.

		Waste Package Dimensions		Footprint per WP, m		# of WPs*	Summed WP area, km ²		
PWR	BWR	Length, m	Diameter, m	Horizontal	Vertical		Horizontal	Vertical	
4	9	5	0.82	4.10	0.53	82583	0.339	0.0436	
12	24	5	1.29	6.45	1.31	28792	0.186	0.0376	
21	44	5	1.60	8.00	2.01	16157	0.129	0.0325	
32	68	5	2.00	10.0	3.14	$^{\sim}10000$	0.100	0.0314	

Table A-2. Total Plan Cross-Sectional Area of Waste Packages

* For a 140,000 MT repository

The calculations in Table A-2 do not include the effect of the borehole diameter, which can be implemented by increasing the effective dimensions of the waste packages (Figure A-1). The total waste package cross-sectional areas accounting for boreholes from 8 to 13 inches in diameter are given in Table A-3 and illustrated in Figure A-2. The effect of borehole diameter is greater for the smaller waste packages because the relative change in the waste package crosssectional area is greater. The effect is greater for vertical emplacement for the same reason. Including the borehole diameter significantly increases the waste package cross-sectional areas (adjusted or "apparent" areas in Figure A-2) and probabilities of intersection. For verticallyemplaced 4PWR/9BWR waste packages, the probability of intersection increases by 56% for the 8-inch boreholes and by 97% for 13-inch boreholes, relative to the unadjusted value (comparing Tables A-2 and A-3). For horizontally emplaced packages the increase is smaller. For 32-PWR size packages, including borehole diameter increases the probability of intersection by 21% (8 inch) to 36% (13-inch) for vertical emplacement, and 7.2% to 12% for horizontal emplacement.

Figure A-2. Change in Total Waste Package Cross-Sectional Area ("Apparent") as a Function of Borehole Diameter: for (left) Horizontal Emplacement, and (right) Vertical Emplacement

Waste Package		# of WPs*	Borehole Diameter,	Adjusted Cross-Sectional Area, m ² /package		Total Adjusted Cross- Sectional Area, km ²			
PWR	BWR		in.	Horizontal	Vertical	Horizontal	Vertical		
4			$\boldsymbol{0}$	4.10	0.53	0.339	0.044		
			8	4.70	0.82	0.388	0.068		
			9	4.78	0.86	0.395	0.071		
	9	82,583	10	4.86	0.91	0.401	0.075		
			11	4.93	0.95	0.407	0.078		
			12	5.01	0.99	0.414	0.082		
			13	5.09	1.04	0.420	0.086		
			$\boldsymbol{0}$	6.45	1.31	0.186	0.038		
	24	28,792	8	7.10	1.75	0.204	0.050		
			9	7.18	1.81	0.207	0.052		
12			10	7.26	1.87	0.209	0.054		
			11	7.35	1.93	0.212	0.056		
			12	7.43	2.00	0.214	0.058		
			13	7.52	2.06	0.216	0.059		
		16,157	0	8.00	2.01	0.129	0.032		
			8	8.68	2.55	0.140	0.041		
	44		9	8.77	2.63	0.142	0.042		
21			10	8.85	2.70	0.143	0.044		
			11	8.94	2.77	0.144	0.045		
			12	9.03	2.85	0.146	0.046		
			13	9.12	2.93	0.147	0.047		
			$\boldsymbol{0}$	10.00	3.14	0.100	0.031		
			8	10.72	3.81	0.107	0.038		
			9	10.81	3.90	0.108	0.039		
32	68	10,000	10	10.91	3.99	0.109	0.040		
			11	11.00	4.08	0.110	0.041		
			12	11.09	4.17	0.111	0.042		
			13	11.18	4.26	0.112	0.043		

Table A-3. Effect of Borehole Diameter Adjustment on Waste Package Cross-Sectional Area

* For a 140,000 MT repository

A.3.2 Statistical Distribution of the Number of Intersections

As noted above, for any given borehole frequency (boreholes/ km^2) the expected number of borehole-waste package intersections is independent of repository size or layout. The expected value does not change with waste package spacing, because an increase in waste package spacing results in a proportionally larger repository footprint, hence, more boreholes are drilled (for a given borehole frequency).

While the *expected* number of intersections does not depend on repository size or layout, the spatial distribution of boreholes is random, and the statistical range of the number of intersections does depend on repository layout. For probabilistic performance assessment this range could be important, so the statistical distribution of the number of borehole/waste package intersections is developed here, based on a given number of boreholes drilled.

The approach uses the layout area assigned to each waste package in the repository (i.e., singlepackage layout area) and applies the binomial distribution. Thus, using the probability of intersection for a single borehole within the layout area for a single package (Table A-4), the binomial distribution represents the probability for a given number of intersections, for a specified number of boreholes drilled. The probability mass function (PMF) for a binomial distribution is defined as:

$$
f(k; n, p) = Pr(K = k) = {n \choose k} p^{k} (1-p)^{n-k}
$$
 Eq. A-1

For $k = 0, 1, 2, \dots$ n, where

$$
\binom{n}{k} = \frac{n!}{k! (n-k)!}
$$

As applied here, *n* is the total number of boreholes within the repository footprint, and *p* is the probability of intersection for any one borehole drilled within the layout area for one waste package (Table A-4). The PMF provides the probability of getting *k* intersections for *n* boreholes. Note that *n* is an integer. It is not possible to drill a partial borehole, so the predicted number of intersections is conservatively rounded up. For small numbers of boreholes the effect of this rounding can be significant as discussed below.

As an example calculation, consider the statistical distributions for the number of intersections for the sedimentary case (single-package layout area $= 900 \text{ m}^2/\text{package}$) and the hard rock case (1,400 m 2 /package). The calculation is done for 32-PWR size packages, and boreholes with 8 and 13-inch diameter (bounding the range considered). The parameters used are shown in Table A-4. Figure A-3 shows PMFs for the number of intersections, using the maximum borehole frequencies from 40 CFR 191 (Section A.2 above). For the sedimentary repository case with horizontal emplacement the PMF peaks at 3 intersections, but 8 intersections will occur more than 1% of the time. For vertical emplacement the most probable number of intersections is 1, and greater than 4 intersections will occur less than 1% of the time. In the hard rock case the probability of no intersections is 72% for horizontal emplacement and 88% for vertical emplacement.

Figure A-3. Probability Mass Functions for the Number of Intersections with 32-PWR Size Packages, for: (left) the Sedimentary (Salt) Repository Case (30 boreholes/ km^2), and (right) the Hard Rock (Crystalline) Repository Case (3 boreholes/km²)

The expected number of intersections can be calculated from the PMFs by summing the product of the probability of occurrence (*y*-axis) multiplied by the number of waste packages intersected (*x*-axis):

Expected number =
$$
\sum_{0}^{n} f(k; n, p) \times k
$$
 Eq. A-2

It might be anticipated that the expected number of intersections calculated this way would be equal to the simple estimates discussed in Section A.3.1 (Table A-3). This is true only when the total number of boreholes calculated from the repository footprint is an integer. In general, the calculated total number of boreholes will not be an integer and will have to be rounded up for use with the binomial distribution. Accordingly, the expected number of intersections from Eq. A-2 will not be equal to the expected numbers based on cross-sectional areas in Table A-3, but will vary as a function of the rounding error. The rounding effect can be quite significant for small numbers of boreholes. To illustrate this, the single-package layout area (for horizontally emplaced 32-PWR size packages, or BWR equivalent) was varied from 35 m^2 to 3000 m^2 with a borehole frequency of 1 borehole per km^2 , to show the possible effect from rounding the number of boreholes (Figure A-4). The effect of rounding can be significant in a relative sense, for small numbers of boreholes drilled, but it decreases rapidly as the number of boreholes increases. Once the repository total layout area is large enough that the expected number of boreholes drilled is 10 or greater, the potential discrepancy in the expected number of intersections is 0.1 or less (Figure A-4). This threshold would be met many times over for a repository in sedimentary or hard rock, for the U.S. SNF inventory (e.g., Table A-4 which describes a repository for SNF in 32-PWR size packages).

Note: The red line represents the expected probability of intersection calculated from total crosssectional area of the waste packages. Borehole frequency = 1 borehole/km². The representative area is the single-package layout area.

Figure A-4. Effect of Rounding Up the Number of Boreholes Drilled to the Next Integer for the Binomial Distribution.

A.3.3 Effect of Repository Layout Size

As noted earlier, for a given borehole frequency (boreholes/ $km²$) the expected number of intersections, which corresponds to the mean of the PMF, will not change with waste package spacing because an increase in waste package spacing results in a proportionally larger repository footprint, and hence, more boreholes drilled. The PMF, however, must change as the number of boreholes increases, because there is a non-zero probability that as many as all of the boreholes could intersect waste packages. Because the binomial distribution is a factorial function, the probability decreases rapidly for each additional intersection. As an example, consider the sedimentary repository case, in which the layout area for each waste package is

900 m². While holding the borehole frequency constant at 1 borehole/ km^2 , the single-package layout area for each waste package is varied, changing the repository footprint, and hence the number of boreholes intersecting the footprint (Table A-5). Single-package layout areas were chosen to result in an integer number of boreholes, to avoid the effect of rounding discussed in previously. As the number of boreholes changes from 1 to 64, the probability of intersecting 0 waste packages changes from 89.00% to 89.58%; the probability of intersecting one waste package changes from 11.00% to 9.87%; and the probability of intersecting 2 waste packages changes from 0% (for the 1 borehole case) to 0.54%. It is clear that changing the single-package layout area (i.e., spacings between waste packages) changes the number of boreholes drilled but will have only a minor effect on the shape of the PMF.

Table A-5. Effect of Repository Layout Size on the PMF for Borehole–Waste Package Intersections (1 borehole/km², 11 inch borehole diameter, horizontal emplacement, 32-PWR size packages).

Layout Area per WP, m ²	100	200	400	800	1600	3200	6400
Total Repository area, km ²	$\mathbf{1}$	$\overline{2}$	4	8	16	32	64
# of Boreholes (at 1 borehole/km ²)	1	$\overline{2}$	4	8	16	32	64
# of Intersections (n)			PMF: Probability of Intersecting n Packages				
0	0.8900	0.8930	0.8945	0.8952	0.8955	0.8957	0.8958
1	0.1100	0.1039	0.1012	0.0998	0.0992	0.0988	0.0987
$\overline{2}$		0.0030	0.0043	0.0049	0.0051	0.0053	0.0054
3			0.0001	0.0001	0.0002	0.0002	0.0002
4			5.71E-07	2.37E-06	3.74E-06	4.56E-06	5.00E-06
5				2.64E-08	6.21E-08	8.80E-08	1.03E-07
6				1.84E-10	7.88E-10	1.37E-09	1.75E-09
$\overline{7}$				7.32E-13	7.79E-12	1.75E-11	2.49E-11
8				1.28E-15	6.07E-14	1.88E-13	3.06E-13
9					3.73E-16	1.73E-15	3.27E-15
10					1.81E-18	1.37E-17	3.10E-17

In a second example, consider the sedimentary and hard rock cases (Section A.2). If we assume the same borehole frequency of 1 borehole/ km^2 , then these two cases are equivalent except for waste package spacing and repository size; there will be 9 boreholes through the repository in the sedimentary case (9 km^2) , and 14 boreholes for the hard rock case (14 km^2) . The PMFs for the number of intersections are shown in Figure A-5. For the sedimentary case the most likely number of intersections is zero, and that will occur about 90% of the time for horizontal emplacement, and about 96% of the time for vertical emplacement. The second most probable number of intersections is 1, and there is a small chance of 2 intersections, especially for horizontally emplaced packages (-0.5%) . Because the largest waste package is being evaluated, the effect of different borehole diameters is small. The results for the hard rock repository are almost identical to the sedimentary results, since as discussed earlier, the expected number of waste packages intersected, which corresponds to the mean of each distribution, must be the same. The change in the number of boreholes (from 9 to 14) slightly changes the shape of the curves, but the change is small. For instance, for horizontal emplacement in a hard rock repository, the probability of one intersection is 0.04% lower than in the corresponding sedimentary cases, and the probability of two intersections is about 0.02% greater. Small differences occur in the low-probability tails of the curves as well.

Figure A-5. Probability Mass Functions for the Number of Intersections at a Borehole Frequency of 1 borehole/km², for the Sedimentary (Salt) Repository Case

The foregoing sensitivity analysis of two parameters (borehole frequency and repository size), which could affect the number of boreholes drilled, shows that they have very different effects on the statistical distribution for the number of intersections. When the borehole frequency (boreholes/ km^2) is increased, the PMFs for number of intersections shift to higher values and broaden (Figure A-3); however, when the repository size is increased without changing the borehole frequency there is little change in the PMF (Table A-5 and Figure A-5).

A.3.4 Effect of Changing Waste Package Size

The foregoing analysis has shown that the repository layout size has little effect on the expected number of waste package intersections, and would have no effect at all, but for the discretization of the predicted number of boreholes, a step necessary to generate the PMF. (Note that this result is specific to the problem formulation where the borehole frequency is established *a priori*, for example by regulation.) Repository geometry also has little effect on the PMFs and cumulative distribution functions (CDFs) for the number of intersections. The parameters of importance to the number of intersections are the borehole frequency (boreholes/km²) and the total crosssectional area of the waste packages (adjusted to account for borehole diameter).

This section evaluates the effect from using different size waste packages in the sedimentary and hard rock cases while keeping all other parameters the same. A borehole frequency of 30 boreholes/km² is assumed for the sedimentary case, and 3 boreholes/km² for the hard rock case. Borehole diameter is assumed to be 11 inches. The single-package layout area is held constant, so comparisons are best limited to similar packages, for example, between 21- and 32- PWR sizes. Changing the waste package capacity while maintaining the same single-package layout area means that the total repository footprint area will change. Table A-6 lists the total

area of the repository and the estimated number of boreholes drilled within the repository footprint at the assumed borehole frequency, for the sedimentary and hard rock cases.

The results for the sedimentary rock repository are shown in Figure A-6. As expected, the smaller and more numerous the waste packages, the more intersections are predicted. For vertical emplacement the expected number of intersections varies from 2.35 for 4-PWR size packages, to 1.17 for 32-PWR size waste packages. For horizontal emplacement the expected number of intersections varies from 12.2 for the 4-PWR package, to 3.50 for the 32-PWR package. The results for the hard rock repository are shown in Figure A-7. The expected number of intersections for vertical emplacement varies from 0.235 to 0.117, and for horizontal emplacement from 1.22 to 0.350, for the 4-PWR and 32-PWR size packages, respectively.

WP Size PWR/BWR	# of WPs	Host Rock Type	Single-Package Layout Area, m^2/WP	Total Repository Area, km ²	# Boreholes Drilled	
4/9	82,583	Sed. (salt)	900	74.32	2,230	
		Hard Rock	1,400	115.62	347	
12/24	28,792	Sed. (salt)	900	25.91	778	
		Hard Rock	1,400	40.31	121	
21/44		Sed. (salt)	900	14.54	437	
	16,157	Hard Rock	1,400	22.62	68	
		Sed. (salt)	900	9.00	270	
32/68	10,000	Hard Rock	1,400	14.00	42	

Table A-6. Total Repository Area for the Sedimentary (Salt) and Hard Rock Cases Assuming that the Single Waste Package Layout Area is the Same for Different Package Types

Figure A-6. Probability Mass Functions (left) and Cumulative Distributions (right) for the Sedimentary (Salt) Repository, with Waste Packages in: (upper) Vertical; or (lower) Horizontal Orientation

Figure A-7. Probability Mass Functions (left) and Cumulative Distributions (right) for the Hard Rock (Crystalline) Repository, with Waste Packages in: (upper) Vertical; or (lower) Horizontal Orientation

Larger waste packages result in fewer borehole/waste package intersections, other factors held constant. However, the different waste load of each container must also be considered. This is done by evaluating the expected number of SNF assemblies exposed in each case. This is equal to the sum of the products of the probabilities of a given number of waste packages being intersected and the number of assemblies in each waste package:

Expected $#$ Assemblies Exposed $=$

Expected Number of Intersections
$$
\times \#
$$
 Assemblies per WP Eq. A-3

The results for the sedimentary repository case are shown in Table A-7. Although the expected number of waste packages intersected decreases with increasing waste package size, more SNF assemblies are exposed. The results for the hard rock case (Table A-8) are consistent.

Note that the relative importance of waste package intersection versus the number of assemblies exposed is not known, and may depend on radionuclide transport details of the human intrusion scenario, the timing of borehole intersection, and the waste isolation performance objectives given by regulation. If intersection of even a single waste package of any size is sufficient to exceed the performance objectives, then larger packages are beneficial. If the quantity of SNF exposed by borehole intersections is critical, then smaller packages are beneficial.

A.3.5 Other Repository Geometries

The general trends presented here are applicable to repository geometries, such as multi-level repositories, with modifications to account for single waste package layout area and total repository area. For instance, assume a two-level repository, for which two cases might be considered:

- Waste packages in each layer are interspersed between those in the other layer. This might be done to provide maximum spacing for thermal considerations. In this case, the single-package layout area and the repository footprint are smaller (half that for a single layer) but the summed waste package cross-sectional area is the same. For a given borehole frequency the expected number of intersections would be the same as for the single-layer case. However, there would be half as many boreholes so there would be slight differences in the PMF for the number of intersections (for example, Table A-6).
- Waste packages in each layer are aligned vertically. For instance, waste packages could be emplaced vertically in large-diameter boreholes (two to a borehole) drilled from underground galleries, with salt backfill between them. Here, the layout area for each pair of waste packages is the same as for one package in the single-layer case, and the repository footprint is half that of the single layer case. The total waste package crosssectional area is also half that of the single-layer case. Hence, the calculated number of intersections would be half that of the single-layer case but each intersection would be with two packages, exposing twice as many fuel assemblies. Therefore, the expected number of package intersections (and the expected quantity of fuel exposed) would be exactly the same as for the single-layer case. The PMF would differ, however, so that the probability of zero intersections would be greater, and intersections with odd numbers of waste packages would not be predicted.

A.4 Conclusions

This analysis evaluates the number of waste packages that might be inadvertently intersected by boreholes, should SNF waste repositories be situated in sedimentary basins or hard rock (represented by crystalline rock for this analysis). The analysis is based on *a priori* borehole frequency, such as that specified in 40 CFR 191 for sedimentary and crystalline rock settings.

The expected number of borehole/waste package intersections at a borehole frequency of 1 borehole/km² is equal to the total cross-sectional area of waste packages in a square kilometer, divided by 1 km². The expected number of intersections at any borehole frequency can be found by multiplying the frequency (in boreholes per $km²$) by this result.

For a given number of boreholes drilled within the repository footprint, a binomial distribution can be used to calculate the probability mass function for the number of intersections. However, the expected number of intersections calculated from the total waste package cross-sectional area is not preserved because of rounding of the total number of boreholes. This effect is significant only when small numbers of boreholes (e.g., fewer than 10) are considered.

The most important parameters affecting the number of waste package intersections are the borehole frequency (boreholes/ km^2) and the waste package geometry (total waste package crosssectional area). The expected number of intersections varies linearly with the borehole frequency. The waste package cross-sectional area defines the size of the "target" and is adjusted to account for borehole diameter (e.g., up to 13 inches). This results in significantly more intersections, especially for smaller waste packages. Minimizing waste package cross-sectional area by using vertical emplacement can substantially decrease the number of borehole intersections. For a given total repository inventory and borehole frequency, use of larger waste packages results in fewer borehole intersections. However, the quantity of SNF exposed by borehole intersections is greater with larger packages, other factors held constant.

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It is notable that repository geometry has little impact on the expected number of borehole-waste package intersections. For a given borehole frequency (boreholes/ km^2), increasing waste package spacing decreases the probability of intersecting a waste package within the single-package layout area assigned to that package, but this is exactly offset by the increase in total repository area, and hence, the total number of boreholes drilled. Increasing the repository area does have a slight effect on the probability mass function for the number of intersections.

It can be concluded that, for repositories in sedimentary rock (e.g., salt) the probability of at least one borehole/waste package intersection is significant. For hard rock (crystalline) repositories the probability is an order-of-magnitude less. Comparing the largest and smallest waste packages analyzed (32-PWR and 4-PWR sizes, or BWR equivalents) the expected number of intersections decreases for larger packages, but the expected quantity of fuel exposed increases (e.g., a factor of 2 greater).

Finally, it should be noted that this analysis has not considered the timing of human intrusion, or the pathway and processes by which radionuclides could be released to the environment.