Features, Events, and Processes Prioritization for Deep Borehole Disposal Concepts in Crystalline Rock and Shale

Ethan Bates,* John Midgley*

*Deep Isolation 2001 Addison St, Suite 300 Berkeley, CA 94704, ethan@deepisolation.com

INTRODUCTION

With current drilling technology, deep borehole repositories could be constructed in a wide range of geological environments, depths, and configurations, increasing siting options and flexibility for nuclear waste management programs. A key component supporting the evaluation of the safety and feasibility of a deep borehole repository is a complete and detailed documentation of the phenomena, initiating events, and boundary conditions included within the long-term performance assessment. Due to the long time periods and wide range of natural and engineered barrier materials and properties encompassed by a repository, the scope of phenomena affecting performance is substantial. These phenomena are organized using a postclosure feature, event, and process (FEP) analysis; and can be managed and evaluated using a systematic screening process to focus on risk-important items. This scope increases where the conceptual design considers multiple waste forms (e.g., Cs/Sr capsules [4], spent nuclear fuel [1, 2], vitrified waste [3]) in a range of geologic media (e.g., crystalline basement, shale, and others) and borehole configurations (vertical, horizontal, deviated). This paper provides an initial highlevel identification and prioritization of FEP groups to support the feasibility evaluation of deep borehole concepts in both crystalline rock and shale. Initial findings are presented on the high-priority FEP groups in these host rocks. This first assessment provides a foundation for deep borehole FEP analyses to support future safety assessments and focus future research for a variety of deep borehole repositories.

FEP PRIORITIZATION

Method

Sandia National Laboratories' existing deep borehole disposal (DBD) post-closure safety analysis and FEP list/screening evaluation [4],[5] provided the starting point for this work. The Sandia FEP analysis was based on the following:

Features

- Waste form and waste package
- Emplacement zone workings
- Seals and plugs
- Host rock, disturbed rock zone (DRZ) and overlying geologic units
- Biosphere

Processes

- Thermal
- Mechanical
- Hydrological
- Chemical
- Biological
- Radiological
- Transport (radionuclide)
- Geologic
- Climatic
- **Events**
- Criticality
- Seismic
- Igneous
- Human Intrusion

For the Sandia deep borehole FEP analysis, a detailed FEP list was developed; the potentially relevant phenomena were represented by a process or event acting upon or within a feature. Preliminary screening of those detailed FEPs was performed for the specific application of Cs/Sr capsule disposal in the deep crystalline basement (at depths >3 km).

To support the preliminary evaluation of multiple waste forms, geologic media, and borehole configurations considered in this paper, the detailed Sandia FEP list was categorized into broader FEP groups, to allow for a more streamlined prioritization process.

The broader FEP groups were constructed from the potential effects of the thermal-hydrological-mechanicalchemical-biological-radiological (THMCBR) processes and the external events affecting the features. THMCBR effects include, for example: barrier material dissolution, degradation, and alteration; heat transfer; fluid flow; gas generation; radionuclide decay and ingrowth; and radionuclide transport (advection, diffusion, colloidal).

The resulting FEP groupings were not completely exhaustive, but they are sufficiently comprehensive for the purposes of prioritizing future research. The broad FEP groups are summarized below:

- Waste form dissolution
- Waste package failure
- Gas generation in the emplacement zone
- Thermal effects (boiling, buoyant flow) in the emplacement zone and overlying seals
- Microbial activity in the emplacement zone and overlying seals
- Seal and plug degradation
- Radionuclide decay/ingrowth

- Radionuclide transport through the DRZ
- Radionuclide transport through the host rock and overlying geologic units
- Radionuclide transport and uptake in the biosphere

These FEP groups were assessed individually in terms of the current state of knowledge and perceived importance to DBD post-closure safety analysis to support deep borehole repository concepts in crystalline rock and shale.

RESULTS

Prioritization of FEP Groups

In deep borehole concepts the greater depth of disposal and decreased influence of near surface processes (e.g., erosion, glacial effects, etc.) means that the host lithology and overlying geologic units (i.e., the natural barriers and their corresponding radionuclide transport behaviors) are relied on for safety to a higher degree in general than for mined repository concepts [1]. Thus, FEP groups related to the natural barriers, whose properties and behaviors vary with depth and drilling processes, were deemed as "high priority" to advance the generic feasibility and safety assessment of DBD concepts.

The safety significance of the seals and plugs in deep boreholes is also considered "high priority". Recent assessments suggest that long-term waste isolation can be achieved, even with conservative assumptions regarding seal degradation [1],[2]. For some mined repositories in crystalline or shale host rocks, the performance of seals, plugs, and engineered components (e.g., buffers, canisters) are relied upon to higher degrees for safety. To address questions in this regard for deep borehole repository concepts, further evaluation of seal and plug degradation phenomena and their impact on safety is needed.

Table I summarizes these high-priority FEP groups and identifies suggested areas for future work for the highpriority FEP groups. Key characteristics of the host rock units, their importance to radionuclide transport, and their interactions with seals and plugs and the DRZ are discussed in the following section.

FEP groups where the potential importance differs depending on the geologic media were deemed "medium priority". Medium-priority FEP groups and associated areas for additional research are summarized in Table II.

Matrix diffusion is a specific detail of radionuclide transport, that may be particularly important for crystalline host rock with advective flow through fractures.

High rates of gas generation may affect engineered barriers so this would be assessed on the same time frame as the safety function of the seals and plugs. Due to the higher hydrostatic pressure associated with DBD emplacement zones, gas generation may be somewhat mitigated through dissolution. The gas generation FEP group was deemed to be medium priority as there are large differences in gas transport behavior between crystalline rock and shale environments.

Biosphere models (including pumping and dilution assumptions) are dependent on emplacement zone depth, the host rock, and the overlying lithologies; they can have an important impact on the post-closure safety assessments.

TABLE I. High priority FEP groups and proposed areas for additional work

FEP group(s)	Areas for additional work		
Radionuclide	-Emplacement zone borehole integrity		
transport	assessments		
through the	-Review of carbon capture and		
host rock and	sequestration (CCS) and mined		
overlying	repository performance assumptions		
geologic units	for shale as a caprock or emplacement		
	zone, respectively.		
Seal and plug	-Sensitivity analysis		
degradation	-Review applicability of seal		
	evolution and degradation models		
	from mined repositories and CCS to		
	DBD conditions		
Radionuclide	Sensitivity analysis of the DRZ in the		
transport	context of repository performance,		
through the	development of more detailed models		
disturbed rock	for DRZ properties (based on risk		
zone (DRZ)	importance).		

TABLE II. Medium priority FEP groups and proposed areas for additional work

FEP group	Proposed areas for additional work
Radionuclide transport (matrix diffusion) in the host rock	Review of applicability of existing matrix diffusion studies
Gas generation in the emplacement zone	Review of potential gas generation sources, calculation of envelope for gas generation and dissolution
Radionuclide transport through the biosphere	Review of biosphere models for various geology types

Host Rock Units- Depth Dependence and Key Transport Properties

A distinguishing feature of DBD is the increased depth of disposal compared to mined repository concepts; thus, understanding the depth dependence of host rock properties is a fundamental task to support the host rock and overlying rock FEP group. Furthermore, quantifying the undisturbed rock hydraulic properties should be done before the full extent of the disturbance due to drilling (i.e., the disturbed rock zone; DRZ) can be assessed. Lastly, the risk significance of both the DRZ and the seals depends on the hydraulic resistance contrast between the DRZ/seals and the host rock [6], which is likely a function of the mechanical boundary conditions imposed by the surrounding host rock [7].

In terms of crystalline rock, a widely acknowledged trend [8] is the reduction in bulk permeability as a function of depth. Additionally, due the effect of dissolved salts and hydrolysis [9], fluid densities are expected to increase with depth (at depth generally $>\sim$ 1-2 km) from \sim 50 to \sim 200 kg/m³. Such increases promote density stratification that acts against vertical advective flow from natural convection [6].

Figure 1 compares four permeability correlations and places them in the context of a recent conceptual DBD repository performance assessment [1] which utilized the Achtziger [10] correlation and accounted for the salinity increase vs. depth.



Fig. 1. Comparison of correlations of crystalline rock permeability vs. depth from Stober and Bucher [10], Achtziger [10], Laxemar data [12], Manning and Ingebritsen [13]

The performance assessment [1] suggests the about two order of magnitude permeability decrease from ~ 10^{-15} m² to ~ 3×10^{-17} m² (and salinity increase) by a depth of ~1.5 km would be sufficient to ensure diffusion-dominated transport from the borehole emplacement zone. This is supported by the natural analogue and isotopic studies conducted at the UPH-3 crystalline basement borehole in Illinois [14] that shows a salinity gradient consistent with stagnant diffusion (not advection) transport at a very similar depth (1.6 km). This is in contrast to mined crystalline repositories where flow and transport from the repository to the biosphere occurs primarily through advection in highly conductive fractures (i.e., fast pathways) which results in more safety reliance on engineered barriers such as the canister and buffer [15].

Clay, shale, and argillite lithologies considered ideal for repository construction would include features such as: rich (~50% content) in clay minerals (mainly smectite and illite); fine grained; lightly indurated [16]. In the context of such shales, DBD repository performance trends are aligned with those for mined repositories in that transport is expected to be diffusion dominated due to the extremely low permeability and the relatively low strength that leads to plastic deformation [12],[17] in these rocks. Table III summarizes the permeability of various clay and argillite rocks studied for mined repositories (typically <500 m depth). At the greater burial depths considered for DBD (>1 km), the host rock clay could be less porous [18] and more indurated (i.e., diagenetically modified) [16]. For depths and temperatures up to 2 km and 70 °C, research suggests that compaction is primarily a mechanical effect. At even greater temperatures/depths a smectite to illite transition causes further changes in properties [19].

TABLE III. Summary of permeabilities from four major underground research labs (URLs) for clay repositories, sorted by age [11]

	Mol	Bure	Mont Terri	Tourn- emire
Country	Bel- gium	France	Swit- zerland	France
Formation	Boom Clay	Callovo- oxfordian argillite	Opalinus clay	Toarcian argillite
Age	30 Ma	155 Ma	170 Ma	185 Ma
Depth (m)	233	495	250-320	250
Permea- bility (m ²)	2.4 ×10 ⁻¹⁹	5×10^{-21} to 5×10^{-20}	2.4 × 10 ⁻²⁰	10 ⁻²² to 10 ⁻²¹

Due to clay and argillite's low overall permeability, preferential fluid flow would occur in the fractures created in the DRZ, but that is expected to undergo self-sealing over time as part of the mechanical behavior of the clay [12]. On the other hand, such low permeability (e.g., 10^{-22} m²) increases the relative importance of assessing gas generation. Shales can fracture depending on how fast the gas pressure increases [12]; however, some studies [20] suggest that gas leakage can occur without creating a path for water flow.

Under diffusion dominated transport conditions, the minimum host rock thickness needed to achieve isolation has been evaluated to be 100 m to 150 m, [17],[21] However, these estimates were derived for conceptual designs, and a license application has not yet been submitted to regulatory authorities for a shale-hosted repository. Development and implementation of clay-based repositories is considered to be at an earlier stage than crystalline mined repositories [12]. Furthermore, there are challenges for obtaining experimental data on these rocks due to their fine-grained nature [18], which commonly leads to sample alteration during core retrieval.

CONCLUSION

This paper presents the results of a FEP prioritization exercise to guide future research efforts for advancing the feasibility and post-closure safety assessments of DBD conceptual designs covering a range of environments, depths, and configurations. The prioritization is based on a judgment of the current state of the art and the importance of identified FEP groups to long term performance assessment. It is concluded that radionuclide transport through the host rock and overlying geologic units, seal and plug degradation, and radionuclide transport through the DRZ are high-priority areas for additional analysis to support DBD concepts in a wider range of host rocks and configurations.

This paper also presents early findings on the high priority FEP group related to host rock properties, which are unique in DBD concepts because of the variation that occurs with depth. Deep crystalline host rock isolation features (permeability, pore fluid salinity and density, etc.) show a clear correlation with depth. At a certain depth, stagnant pore fluid conditions result in diffusion as the primary transport mechanism. More investigation and additional data are needed to draw general correlations about the depth variation of clay properties; however, this initial overview suggests that stress, age, and geological history are important additional drivers to consider.

ACKNOWLEDGEMENTS

The authors acknowledge the valuable guidance, contributions, and expertise that Geoff Freeze, David Sassani, Tara LaForce, and Patrick Brady provided to this work. Rich Muller and Stefan Finsterle also contributed as reviewers and their efforts are appreciated.

REFERENCES

1. S. FINSTERLE ET AL., "Post-Closure Safety Analysis of Nuclear Waste Disposal in Deep Vertical Boreholes," *Energies*, **14**, 19 (2021).

2. S. FINSTERLE, ET AL., "Sealing of a Deep Horizontal Borehole Repository for Nuclear Waste," *Energies*, **14**, 1 (2021).

 M. J. RIGALI, S. PYE, E. HARDIN, "Large Diameter Deep Borehole (LDDB) Disposal Design Option for Vitrified High-Level Waste (HLW) and Granular Wastes.," SAND2016-3312, Sandia National Laboratories (2016).
 G. A. FREEZE, ET AL., "Deep Borehole Disposal Safety Analysis," FCRD-UFD-2016-000075, Rev. 0, Sandia National Laboratories (2016).

5. G. A. FREEZE, ET AL., "Deep Borehole Disposal Safety Case," SAND2019-1915, Sandia National Laboratories (2019).

6. E. A. BATES, "Optimization of deep boreholes for disposal of high-level nuclear waste," Ph.D. Thesis, Massachusetts Institute of Technology (2015).

 E. A. BATES, ET AL., "Mechanical Stresses Affecting Deep Borehole Disposal of High-level Nuclear Waste," *Proceedings of the 22nd Int'l Conference on Nuclear Engineering (ICONE22)* Prague, Czech Republic (2014).
 E. A. BATES, ET AL., "Can deep boreholes solve America's nuclear waste problem?," *Energy Policy*, **72** (2014).

 P. BRADY, C. LOPEZ, D. SASSANI, "Granite Hydrolysis to Form Deep Brines," *Energies*, 12, 11, (2019).
 P. ACHTZIGER-ZUPANČIČ, S. LOEW, G. MARIÉTHOZ, "A new global database to improve predictions of permeability distribution in crystalline rocks at site scale," *J. Geophys. Res. Solid Earth*, 122, 5 (2017).
 I. STOBER, K. BUCHER, "Hydraulic properties of the crystalline basement," *Hydrogeol. J.*, vol. 15, 2 (2007).
 C. TSANG, I. NERETNIEKS, Y. TSANG, "Hydrologic issues associated with nuclear waste repositories," *Water Resour. Res.*, 51, 9 (2015).

13. C. MANNING, S. INGEBRITSEN, "Permeability of the continental crust: Implications of geothermal data and metamorphic systems," *Rev. Geophys.*, 37, 1 (1999).
14. R. A. COUTURE, M. G. SEITZ, "Movement of fossil pore fluids in granite basement, Illinois," *Geology*, 14, 10

(1986).
15. P. N. SWIFT, D. SASSANI, "Impacts of Nuclear Fuel Cycle Choices on Permanent Disposal of High-Activity Radioactive Wastes.," SAND2019-5941C, Sandia National Laboratories (2019).

16. E. HARDIN, "Review of Underground Construction Methods and Opening Stability for Repositories in Clay/Shale Media," FCRD-UFD-2014-000330 Rev. 0 Sandia National Laboratories (2014).

17. L. ZHENG, ET AL., "Generic Argillite/Shale Disposal Reference Case," FCRD-UFDC-2014—000319. Lawrence Berkeley National Laboratory (2014).

18. I. C. BOURG, L. E. BECKINGHAM, D. J. DEPAOLO, "The nanoscale basis of CO2 trapping for geologic storage," *Environ. Sci. Technol.*, **49**, 17 (2015).

C. PELTONEN, Ø. MARCUSSEN, K. BJØRLYKKE,
 J. JAHREN, "Clay mineral diagenesis and quartz cementation in mudstones: The effects of smectite to illite reaction on rock properties," *Mar. Pet. Geol.*, 26, 6 (2009).
 C.-L. ZHANG, "Investigation of gas migration in damaged and resealed claystone," *Geol. Soc. Lond. Spec. Publ.*, 415, no. 1 (2015).

21. M. J. HENDRY ET AL., "Can argillaceous formations isolate nuclear waste? Insights from isotopic, noble gas, and geochemical profiles," *Geofluids*, **15**, 3 (2015).