Reference shale host rock properties and chemistries for deep borehole disposal performance modeling

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INTRODUCTION

Deep Isolation is developing a series of long-term performance models to assess the behavior of repository systems containing various types of advanced reactor waste streams in a Universal Canister System (UCS). The UCS is designed to contain a range of advanced reactor waste streams with the option for ultimate disposition in either mined or deep borehole repository configurations. This paper summarizes the early efforts of building the long-term screening performance assessment model which included a review of safety-relevant host rock properties affecting the degradation rate of the waste forms as well as the transport behavior of fluids in the near and far fields of deep borehole repositories.

DESCRIPTION OF WORK

Pore fluid properties

Conditions of a borehole repository disposal zone (including the canister and its immediate vicinity) will change over time based on the integrity of the casing and the composition and rate of intrusion of pore fluids. Because long-term safety calculations will conservatively assume canister failure -allowing for direct interaction of the repository environment with the waste forms- the chemistry of these pore fluids will impact the degradation rate of the waste forms contained in the breached canister. This will subsequently play a role in determining the radionuclide solubilities and transport into the far-field.

Host rock pore fluid chemistry for shale and deep crystalline rock environments are typically reducing, highly saline, and low in oxygen. For example, salinity is highly variable in shale and clay formations with values from <10 g/liter (Boom Clay, Opalinus Clay, Wakkanai mudstone) to over 400 g/liter (Marcellus shale, Bakken shale, Utica shale). Reference conditions for shale and crystalline rock pore fluids reported in prior works is summarized in Table I.

TABLE I. Range of pore fluid chemistry assumptions and measurements relevant to disposal in shale [1], [2] and crystalline rock [3], [4].

Fluid	**Shale**	**Crystalline rock**
Salinity	41-400 g/l	117-350 g/l
pH	7-8	7.5-8.5
Eh	-200 to -300 mV	-100 to -300 mV

Host rock properties

Permeability, porosity, compressive strength and sealing behavior help determine the confining properties of the disposal zone. In regards to shale, relevant hydrogeological and mechanical properties have been extensively studied in the context of oil/gas extraction, carbon sequestration [5], and geologic repositories. For this work, safety relevant shale properties for Dutch [6], French [7], [8], Japanese [9], Swiss [10], [11], [12], and U.S. [13], [14], [15], [16] geologic repositories were reviewed. Typically, these data sources and industries (fossil fuel and nuclear waste disposal) are approached separately, but one valuable reference compiled existing data from the fossil fuel industry [12] and interpreted them in terms of repository analysis. Shales considered for geologic repositories and carbon capture and storage are sealing shales, while shales intended to be hydraulically fractured for oil and gas extraction are distinct and can be categorized as brittle shales on the basis of their lower clay content [5].

RESULTS

Based on the range of conditions reviewed and practical considerations of the properties of the emplacement fluid that can be controlled through the design of the borehole repository, a set of generic chemistry assumptions were developed. Prior to casing the borehole, the borehole will be filled with a drilling mud with a salinity that is similar to the native pore fluids to prevent damage to the host rock. However, after fully casing the borehole, the drilling fluid can be displaced and replaced with an emplacement fluid with properties to manage corrosion (e.g., lower salinity, low oxygen content). Here it is assumed that the fluid salinity could be reduced to 1% of its initial value and pH and Eh are also controlled via standard fluid chemistry control practices to manage corrosion of the casing and canister. Reference conditions for deep borehole repository emplacement fluid are summarized in Table II.

TABLE II. Reference assumptions for initial emplacement fluid and disposal zone chemistry

Parameter	Value	Discussion
Salinity	2 g/l or more	Assumed to be 1% of surrounding pore fluid (with 200 g/l assumed as a reference value for the pore fluid concentration).
pH	>7	Initially controllable through standard oil/gas fluid chemistry control practices.
Eh	<-200 mV	

For the purpose of long-term modeling (after the initial canister breach) the pH and Eh would be determined by the native, intruding pore fluids. In a shale host rock, the pH and Eh appear to be buffered through carbonates and other phases. For example, in situ geochemical studies of the Callovo Oxfordian Clay performed by Andra [7] of waters pumped from a borehole drilled in the near Bure, France, show that Eh values stabilize over time (as oxygen introduced for calibration dissipates) and the nominal values in the host rock return to normal in a range close to -200mV.

Regarding shale host rock transport properties, the following general conclusions were drawn.

- **Permeability:** Tends to range between 10^{-18} m^2 and 10^{-21} m^2, with higher clay content generally correlated with lower permeability.
- **Porosity:** Varies widely from 5-40% with no clear correlation to mineralogy.
- **Mechanical behavior:** Shales with clay fractions greater than ~40% have lower unconfined compressive strength (<50 MPa) and are more capable of self-sealing when fractured, while shales with less clay content tend to be brittle [5]. The type of clay (illite vs. smectite) does not appear to be significant in terms of this general trend of a reduction in mechanical strength of the rock. In a mined repository context, fractures created by excavation could self-heal within as little as 20 years [16], although additional work is needed to support this behavior in deep borehole conditions.
- **Lateral extent of shale formations:** In general, shale formations tend to form in regional basins covering many hundreds to thousands of square miles as seen in a USGS compilation [17]. Hence, for modeling purposes, an essentially 'infinite' lateral thickness shale layer might be appropriate given the relative scale of a repository to geologic formations.

- **Thickness:** Shale formation thickness and depth vary widely from 10s to 100s of meters. This is illustrated in maps of the Mancos Shale [15]. However, thickness and depth values appropriate for hosting a repository (1-3 km depth, >100m thickness) are supported by documented shale deposits across the US.

Recommended ranges for shale properties based on this literature survey are summarized in Table III.

TABLE III. Summary of recommended reference values for confining properties of shale in the depth ranges considered for deep borehole disposal (1-3 km)

Parameter	Value range	Basis
Permeability	10^{-18} m^2 to 10^{-20} m^2	[5], [6], [10], [12], [14], [15], [18]
Porosity	10-40%	[5], [6], [10], [12], [14], [15], [18]
Salinity	>200 g/l	[14], [15], [18]
pH	7-8	[6], [7], [8], [9], [10], [11], [19]
Eh	<-200 mV	[8], [9], [10], [11], [15], [18], [19], [19], [20]
Clay content	>40%	
Unconfined compressive strength	< 50 MPa	For shales with clay content >40%, [5], [14], [15], [18]
Thickness	10-600 m	[14], [15], [16], [18]

CONCLUSION

Establishing realistic modeling input assumptions and uncertainty ranges based on previous data is a key step in developing generic long-term performance projections for deep borehole repositories. This paper reviewed data sources across multiple industries to establish a baseline set of recommendations for these modeling inputs. Some properties, such as shale permeability, vary over more than three orders of magnitude; however, even at the upper end of the range presented here (10^{-18} m^2), a shale formation with a thickness of 500 meters would still represent a relatively hydraulically isolated system capable of impeding fluid flow. Thickness also varies by an order of magnitude. Future performance modeling will complete sensitivity studies to further support the selection of defensible and generic values for modeling generic deep borehole disposal performance, as well as providing insight into site selection criteria for these repositories. Future work may also evaluate the impact of cement chemistry, which also affects radionuclide solubility.

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