SUMMARY REPORT:
WORKSHOP ON BUFFER CONCEPTUALIZATION FOR PERFORMANCE ASSESSMENT

Prepared for

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Prepared by

O. Osidele,[1] J. Gwo,[2] O. Pensado,[1] T. Ahn,[2]
R. Fedors,[2] X. He,[1] C. Manepally,[1] C. Markley,[2]
S. Mohanty,[1] P. Shukla,[1] and S. Stothoff[1]

[1]Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

[2]U.S. Nuclear Regulatory Commission
Washington, DC

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

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1 INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC) and the Center for Nuclear Waste Regulatory Analyses (CNWRA®) staff members participated in a one-day technical workshop on buffer conceptualization for performance assessment held on February 24, 2015, at NRC in Rockville, Maryland and CNWRA® in San Antonio, Texas. The workshop participants included subject matter experts in coupled processes, corrosion, geochemistry, and performance assessment modeling. This workshop was motivated by the need to evaluate potential updates to the NRC's Scoping of Options and Analyzing Risk (SOAR) performance assessment code (Markley, et al., 2011) regarding generic representation of the engineered buffer as a barrier component of the geologic disposal system. Specifically, based on previous reviews and applications of the SOAR code, NRC and CNWRA staff members have noted that explicit connections between buffer performance and environmental conditions at the waste package do not exist. It also was noted that the evolution of the buffer during a thermal period is not considered in the current version of the SOAR code. Preliminary discussions among the performance assessment, coupled processes, and materials corrosion groups have indicated that significant uncertainties remain in knowledge and understanding of processes that could influence buffer and repository performance. In addressing these issues, the goals of the workshop were to

(i) Assess current understanding of buffer performance in the near field of a geologic disposal facility.

(ii) Develop scenarios and conceptualizations of buffer evolution for potential incorporation into the SOAR code, if relevant to repository performance.

As shown in the agenda (Appendix A), the workshop devoted more time and effort to facilitate discussions rather than topical presentations. This approach enabled participants to focus on knowledge integration directed at improving abstraction of buffer-related processes in the SOAR code. Four brief presentations summarized the current state of knowledge on buffer coupled processes, waste package corrosion, geochemical conditions, and performance assessment modeling. Some uncertainties were identified for possible further review. Three facilitated discussion sessions were conducted with the goal of defining a nominal or reference scenario to support developing a generic abstraction of buffer performance. These discussions were framed around the preliminary topics listed in Appendix B, which were developed from a series of workshop planning meetings between NRC and CNWRA staff members. These planning meetings resulted in consensus on basic functions of the buffer, namely, containment and isolation of wastes, control of chemical environment around the waste package, retardation of radionuclide releases, and mechanical stability of tunnels and deposition holes. These functions were reiterated in the brief presentations that preceded the facilitated discussions.

During the discussion sessions, the workshop participants (i) identified key buffer processes; (ii) defined the main elements of a nominal scenario for performance assessment incorporating an engineered buffer; and (iii) identified potential variations of the nominal scenario resulting from elevated temperatures, disruptive events, and climate changes. The workshop concluded with an enumeration of action items for abstraction of a nominal or reference scenario into the SOAR code and agreement on information needs, residual uncertainties, and concepts that require further understanding.

This report summarizes the workshop proceedings in the general order of the agenda, shown in Appendix A. All presentation slides are archived on the NRC-CNWRA SharePoint® site.

2 SUMMARY OF STATE OF KNOWLEDGE AND KEY GAPS

Four presentations were given by CNWRA staff members. These presentations provided a brief summary of the current state of knowledge and key gaps related to buffer coupled processes, waste package corrosion, geochemical conditions, and performance assessment modeling. The presenters highlighted basic functions of the buffer and waste package that were discussed extensively during previous NRC-CNWRA workshops on buffers, coupled processes, and waste package corrosion (Manepally, et al., 2011; He, et al., 2011; Manepally, et al., 2012; Myers, et al., 2012). The subsequent facilitated discussions focused on determining aspects of the current understanding of buffer-related processes that are significant to repository system performance. The main messages from these presentations and key questions on performance assessment for the subsequent discussion sessions are detailed in the following sections.

2.1 Evolution of Environmental Conditions in the Buffer

Two safety functions of the buffer were described: (i) providing isolation and containment and (ii) reducing radionuclide releases. The third function, mechanical stability of tunnels and deposition holes, is implicitly accounted for in performance assessments that dismiss failure of waste packages by mechanical interaction with the host rock. Performance of the safety functions depends on prevailing environmental conditions. The capability of bentonite buffer material to swell and seal gaps and openings when absorbing water is a critical feature of the safety functions of the buffer. Changes in thermal, hydrological, geomechanical, and chemical conditions affect features of bentonite buffer material with implications for buffer and repository performance. The evolution of environmental conditions and impacts on the buffer material can be evaluated by considering four periods:

- **Repository construction and operation period**: This period involves buffer installation and waste emplacement. The initial hydrologic saturation of the buffer material depends on the type of clay and could range from 20 percent for granulated bentonite in the proposed Swiss concept[1] to 80 percent for compacted bentonite blocks in the Swedish concept (SKB, 2011). This is the only period associated with the preclosure timeframe. The remaining periods can be considered postclosure.

- **Thermal period**: Highest temperatures are expected in this period, leading to redistribution of moisture in the buffer. The buffer is likely to be driest at the waste package-buffer interface and wettest at the host rock-buffer interface. Spatial heterogeneity in saturation could result in uneven swelling and shrinkage, which in turn, could lead to the development of microfractures and preferential fast flow paths in the buffer. Another consequence of heterogeneous resaturation could be a situation whereby the outer buffer (closer to the host rock) seals first, thereby slowing further resaturation of the inner parts of the buffer (nearer to the waste package). Chemical processes, such as dissolution, alteration (e.g., illitization at temperatures greater than 100 °C), and precipitation of minerals also are possible during the thermal period and could significantly affect the buffer's swelling capabilities, depending on the thermal load imposed and the resulting extent of the mineralogical change.

[1]<http://www.nagra.ch/en/repositoriesforhlw.htm> (30 June 2015)

- **Post-thermal period**: This period involves slow return to ambient temperatures and pressures, as the thermal load dissipation continues. The resaturation of the buffer occurs, ideally, with an inward progressing front towards the waste package.

- **Long-term period**: During this period, the temperature in the buffer has returned to ambient conditions. If buffer mineralogy was not significantly altered during the prior thermal period, the bentonite buffer functions as designed. Changes to external groundwater chemical composition may lead to erosion of the buffer in crystalline host rocks.

The conceptualization of coupled thermohydrological-mechanical-chemical (THMC) processes and their impact on specific properties was discussed. NRC and CNWRA staffs have been involved in the current phase of the Development of Coupled Models and Their Validation Against Experiments (DECOVALEX) project since 2012. The DECOVALEX project is an international collaboration of modeling teams focused on modeling THMC processes associated with radioactive waste disposal. The project aims to improve the reliability of modeling tools and to exchange lessons-learned in using the tools through comparisons with data from laboratory and field experiments. Part of the current NRC/CNWRA DECOVALEX project involved modeling a column of buffer subject to heating and hydration using the combination of xFlo and FLAC codes (Stothoff, et al., 2015). The modeling efforts provided several insights including (i) the influence of metallic components present in both the engineered barrier system and the experimental apparatus on temperature distribution, (ii) the effect of moisture redistribution on swelling pressures developed in the buffer, and (iii) the possible build-up of air pressure during the thermal period. However, some field experimental data for temperatures above 100 °C suggest that release of pressure may occur through the excavation damaged zone, even though plugs and seals were installed for the tests. In other words, the occurrence and potential magnitude of pressure buildup in the buffer during the thermal period remain uncertain.

Most international waste disposal programs impose a maximum temperature limit of 100 °C in clay buffers to avoid chemical changes that could significantly reduce swelling. Chemical processes that could affect swelling capabilities, such as illitization, occur at temperatures greater than 100 °C. However, some research indicates this temperature criterion is too low (Liu, et al., 2013). This approach is the basis for recent numerical and experimental studies by the U.S. Department of Energy (DOE) Used Fuel Disposition (UFD) Program that focused on bentonite buffers (Jové Colón, et al., 2014). The DOE results from these studies show that high temperature induces illitization, transients in pore pressures up to 10 MPa, water in liquid phase at temperatures up to 200°C, and full saturation of buffer materials in 10 to 20 years. Impacts of elevated pressures and temperatures on corrosion of metals and waste forms could be significant. Studies on behavior of buffer materials under such extreme geologic disposal conditions are rare, thus increasing uncertainty in predictions of repository performance.

For performance assessment, the key questions identified for discussion were:

- How much damage could be inflicted on the buffer and waste package during the four evolution periods, and how might the rates of radionuclide release be affected?

- What is the significance and functional relationship of heterogeneous resaturation, mineralogy changes, and buffer erosion to repository performance metrics, such as waste package lifetime, waste isolation, radionuclide release rates, and radionuclide retardation?

- What periods in the buffer evolution are the most critical to overall system performance?

- What is the risk significance of gas generation and migration processes to repository performance?

- Can elevated gas pressures be established and maintained in the buffer, considering the preconstruction water pressures existing within the host rock at depth?

- Gas buildup appears both detrimental and beneficial to repository system performance. For example, if there is gas buildup, could the ensuing high pressures compromise waste packages thinned by corrosion from contact with high-temperature fluids and dissolved chemical species or due to mechanical interactions? Would high pressures and mechanical forces damage buffer materials? Would high pressures indicate the lack of pathways for gas pressure relief, and therefore also indicate a system that would retain radionuclides or significantly limit their release and transport?

2.2 Waste Package Materials

The presentation on waste package materials identified redox conditions, temperature, and degree of saturation among the factors that determine the rate of waste package corrosion. Other important factors include pore water chemistry, microbial activity, and mechanical loads acting on the waste packages. Technical gaps and results from CNWRA studies were discussed for corrosion of copper and carbon steel because they are the waste package materials proposed for use by several countries using clay buffer material. Potential impacts of hydrogen gas generation, chloride and sulfide on corrosion rates, and passivity also were described.

According to the copper Pourbaix (potential-pH) diagram (Pourbaix, 1974), in oxygen-free environments, copper is thermodynamically stable and general corrosion would be negligible. As such, copper containers would be extremely long-lived for a wide range of host rock types, and the hydrogen generated from copper corrosion would be extremely small. However, some researchers (Hultquist, et al., 2009) have proposed different copper corrosion mechanisms that could lead to higher corrosion rates and equilibrium hydrogen partial pressure. Under oxygen-free conditions, if copper reaction with water is negligible, attack by sulfide derived from mineral dissolution and/or microbial activity is reported to be the main corrosion risk to a copper container (SKB, 2010a). Copper reacts with sulfide forming a copper sulfide film. Studies have shown the structure and properties of the sulfide film have a significant influence on both the mechanism and the rate-limiting step of the corrosion process. Chloride, which is commonly present in groundwater, has been shown to influence copper corrosion by changing the interfacial sulfide film structure and properties. Overall, technical gaps for copper corrosion are mainly focused on three areas: (i) thermodynamic stability of copper and effect of chloride on copper corrosion in oxygen-free pure water, (ii) copper sulfide film passivity in sulfide-containing environments, and (iii) effect of chloride on the interfacial sulfide film.

Copper corrosion studies carried out at CNWRA in simulated groundwater with an oxygen concentration of less than 10 parts per billion (ppb) recorded higher corrosion rates than those currently specified in SOAR under anoxic conditions. The measured corrosion rates are consistent with some literature data where the oxygen concentration was less than 1 ppb (Cleveland, et al., 2014). The corrosion product is predominantly Cu_2O with a small amount of chloride. *Ex-situ* measurement of hydrogen directly generated from copper corrosion in CNWRA studies using gas chromatography is not unequivocally correlated to the copper corrosion rate because of complicating factors such as (i) existing background hydrogen in the autoclave, (ii) low amounts of hydrogen generated that are close to the instrument detection limit, (iii) possibly incomplete oxygen depletion by inert gas deaeration during the tests, and (iv) more complex corrosion mechanisms in chloride-containing solution.

Carbon steel is reported to have low corrosion rates in simulated reducing groundwaters, which makes it possible for carbon steel waste packages to last for thousands of years. Technical gaps for carbon steel corrosion are mainly (i) the magnitude of anaerobic corrosion rates and consequent container failure time; (ii) impacts of corrosion products on the properties of other barriers (e.g., incorporation of iron into the bentonite buffer and effect of hydrogen on the swelling and sealing properties of clay buffers); (iii) passivity in alkaline solution and effects of chloride, sulfide, and thiosulfate on passivity; and (iv) hydrogen generation from corrosion, and associated hydrogen induced cracking. Carbon steel corrosion studies in anoxic alkaline water carried out at CNWRA produced corrosion rates that are consistent with existing corrosion rates input to the SOAR code. Chloride, sulfide, and thiosulfate are found to affect passivity and repassivation of carbon steel. Repassivation studies at open circuit conditions and hydrogen induced cracking tests are underway to address technical gaps.

For performance assessment, the key questions identified for discussion were:

- Is the amount of generated hydrogen enough to cause hydrogen embrittlement of carbon steel packages or to inhibit dissolution of spent nuclear fuel?

- Are scenarios that involve hydrostatic or seismic loading, or welding coupled with hydrogen embrittlement of carbon steel important in assessing the lifetime of waste packages?

- If the carbon steel must be directly exposed to hydrogen during long periods to cause a change in mechanical properties, is such long-term exposure feasible or would hydrogen instead be dispersed into the host rock? If hydrogen is locally contained, would such hydrogen encapsulation be an indication of a tight system that also would isolate radionuclides or significantly delay their release?

2.3 Chemical Conditions at the Waste Package, Spent Nuclear Fuel, and Buffer Interface

The chemical characteristics of water contacting waste packages and the potential impacts on buffer mineralogy and waste package corrosion were presented, based on results of geochemical reactive transport modeling conducted previously at CNWRA (Pabalan, et al., 2012). Computations were performed using geochemistry software OLI Analyzer Studio™ (OLI Systems, Inc., 2012) and Geochemist's Workbench X1t (Bethke, 2008). These computations considered slow diffusion of groundwater into the bentonite buffer material. Bentonite clay is a material that undergoes cationic exchange. As time elapses and groundwater passes through the bentonite, the cationic composition of bentonite will change to eventually equilibrate with the groundwater.

For performance assessment, the key questions identified for discussion were:

- Would a change in ionic composition of bentonite have any influence on waste package lifetime?

- In the event of radionuclide release, would changes in ionic composition of bentonite affect radionuclide mobilization, retardation, and retention in the bentonite clay buffer material?

- Since buffer materials are intended to limit transport of corrosive species (e.g., hydrogen sulfide and chloride ion) to the waste package surface, can waste package corrosion rates be explicitly correlated to the rate of transport of corrosive species, or are corrosive species mostly catalytic activators of corrosion?

2.4 State of Knowledge of Key Issues Related to Buffer and Its Interfaces–A Performance Assessment Perspective

To describe the current state of knowledge of key issues related to the buffer and its interfaces with the waste package and host rock, several recent geologic repository programs that include the buffer as an engineered barrier component were reviewed. The presentation focused on bentonite as a buffer material because it is common to the majority of repository concepts worldwide. Most of the studies on bentonite buffer materials have been conducted at the process level and only a handful of the results obtained have been incorporated into performance assessments to date. Sweden, Finland, and the United States are the latest countries to have completed performance assessments in support of license applications for geologic repositories. The following paragraphs highlight performance assessment modeling approaches adopted by the DOE and the Swedish Nuclear Fuel and Waste Management Company (SKB), and the main processes commonly associated with buffer performance in the U.S. and international repository programs. Some results published by SKB also are examined to provide an understanding of the significance of buffer processes to repository performance.

In the DOE generic repository performance assessment model development activity, the overarching approach is to rely less on conservative assumptions, simplifications, and process abstractions in order to increase transparency and model confidence. As a result, the DOE model (i.e., the PFLOTRAN multi-physics code) has more detailed spatial-temporal geometries and coupled processes representation than is customary for performance assessment models. The model is designed for analyzing a range of disposal options (e.g., repositories sited in salt, granite, or clay host rocks, and deep borehole disposal) and for explicitly calculating THC processes in the buffer. PFLOTRAN models nonisothermal multiphase flow, reactive transport, and geomechanics. Processes, such as heat flow, dispersive transport, soil-matrix compressibility, and hydrogen gas generation sorption isotherms, are included in the model. The model currently does not handle disturbed scenarios. The model includes reference data sets for buffers in repositories sited in salt, granite, and clay/shale host rocks.

SKB’s approach has been to use a simplified performance assessment model with numerous supporting analyses. Also, the SKB model was developed for a specific repository system that features copper waste packages protected by bentonite buffer, situated in crystalline host rock. This combination also is considered in the SOAR performance assessment model. The SKB performance assessment scenarios are structured around a set of safety functions by which a repository component is deemed to contribute to repository safety (SKB, 2011). The primary safety functions support containment by retaining spent nuclear fuel within the waste package. The secondary safety functions support retardation by delaying corrosive material from reaching the waste package and delaying radionuclide release if the waste package fails. For example, one safety function for containment requires that the buffer limits advective transport. A safety function indicator is a measurable or calculable property of a repository component that indicates the extent to which a safety function is achieved. For example, swelling pressure is a safety function indicator for limiting advective transport. A numeric limit, or safety function indicator criterion, is associated with each safety function indicator. For example, to limit advective transport, the swelling pressure of the buffer should not exceed 1 MPa. The impacts of component processes on repository performance are determined by comparing the measured or calculated safety function indicator to its corresponding safety function indicator criterion. In the SKB performance assessment, the nominal scenario is composed of safety function indicators that fulfill their respective indicator criteria, while alternative scenarios are developed by assuming one or more safety function indicator criteria are violated.

Table 2-1 lists the main processes associated with buffer performance and also identifies whether a process is relevant before or after waste package failure. In the SKB performance assessment, only the processes that fulfill safety functions are considered further for impact analysis or inclusion in the performance assessment model. Some processes were eliminated from explicit consideration when those were bounded by other processes. For example, diffusive transport of species that control corrosion rate and radionuclide transport are bounded by advective transport. The table also shows processes that are controlled by buffer design. An implementer will likely put a limit on the sulfide, total sulfur, and organic content in the buffer material, if the impacts of those sources would significantly affect waste package corrosion.

SKB analyzed various processes identified in Table 2-1 for their impacts on waste package performance (SKB, 2010b). Most of the analyses were conducted outside of the SKB performance assessment model, for example using mass balance and bounding calculations. Results of these SKB analyses are presented in Table 2-2, showing potential impacts of key processes and environmental conditions on waste package failure in terms of the depth of waste package damage by corrosion. The table shows the impacts may vary by orders of magnitude. For example, nitric acid formed by gamma radiolysis in the presence of nitrogen and oxygen leads to a corrosion depth of 8×10^{-6} mm over a million years. Bounding calculations with all organics in the buffer being readily available for sustaining microbial processes result in a corrosion depth of 2 mm in 1 million years. Corrosion depths from all bounding microbial process pathways (i.e., through the formation of sulfide) would add up to 3.14 mm (2 + 0.04 + 0.4 + 0.7) in a million years, according to SKB.

Table 2-3 presents results from an SKB analysis estimating potential release from a conceptual repository system that includes the buffer as an engineered barrier (SKB, 2011). The performance metric SKB adopted for this analysis is the near-field release rate (Bq/y), converted to comparable dose equivalent (μSv/y) by applying a constant landscape dose conversion factor (μSv/Bq) for each radionuclide considered in the analysis. The results highlight the significance of buffer performance because the dose equivalent estimated for the analyzed scenarios (or cases) are spread by several orders of magnitude above and below the Swedish regulatory dose limit of 14 μSv/y. Table 2-3 also compares three scenarios that initiate with a large hole in the waste package (Cases 5a, 5b, and 5c). The dose equivalents from these scenarios are normalized relative to Case 5a, which assumes that all waste packages are failed, the buffer is intact, and release into the buffer starts 100 years after repository closure. When the buffer in a few boreholes is assumed failed (Case 5b), the release increases 133 times, suggesting that significant performance can be attributed to the presence of intact buffer material.

Similar to the SKB concept, the SOAR code includes the option to use a bentonite buffer as a component of the engineered barrier system. The SKB performance assessment provides insights into concepts and approaches that may be considered for future development of the SOAR code, particularly in relation to (i) the buffer-waste package interface, (ii) use of safety function indicators to screen specific processes, and (iii) characterizing the significance of the buffer to repository system performance. Results of the SKB performance assessment indicate the buffer is an important barrier to limit the release of radionuclides. The list of buffer processes, shown in Table 2-1, provides a practical starting point for identifying processes to consider for alternative buffer materials, host rock types, waste package materials, and repository environments.

Table 2-1. Processes Commonly Associated With Buffer Performance			
Process	**Note**	**Process**	**Note**
Heat transport	[1]	Transport of radionuclides by a gas phase	[F]
Freezing	[1]	Diffusive transport of species that control corrosion rate and radionuclide transport	[2]
Water uptake and transport in unsaturated conditions	[1]	Alteration of impurities	[3]
Water transport under saturated conditions	[1]	Aqueous speciation and reactions	[3]
Gas transport/dissolution	[1][F]	Radiation-induced transformations	[4][F]
Piping/erosion	[1]	Radiation attenuation/heat generation	[4]
Colloid transport	[1][F]	Liquefaction	[4]
Swelling/mass redistribution	[1]	Radiolysis of pore water	[4]
Advective transport of species	[1]	Material composition	[5]
Montmorillonite transformation	[1]	Iron-bentonite interaction	—
Montmorillonite colloid release	[1]	Osmosis	—
Microbial processes	[1]	Waste-clay interaction	—
Cementation	[1]	Mechanical alteration of clay by gas breakthrough	—
Sorption (including ion exchange)	[1]	Speciation of radionuclides	[F]

Sources:
Manepally, C., R. Fedors, G. Ofoegbu, B. Dasgupta, R. Pabalan, J. Bradbury, K. Chiang, and O. Osidele. "Buffer Workshop Report." San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2012.

SKB. "Buffer, Backfill and Closure Process Report for the Safety Assessment SR-Site." Technical Report TR–10–47. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Co. November 2010b.

Wilson, J., D. Savage, A. Bond, S. Watson, R. Pusch, and D. Bennett. "Bentonite: A Review of Key Properties, Processes and Issues for Consideration in the UK Context." Report QRS-1378ZG-1, Version 1.1. Henley-on-Thames, Oxfordshire: Quintessa Limited. February 2011.

Notes:
[F]: Failed WP
[1]: Processes that fulfill safety functions
[2]: Advective transport bounds this process
[3]: Critical for determining buffer chemistry; no direct impact on safety
[4]: Processes that did not fulfill safety functions (deemed insignificant to long-term safety)
[5]: Buffer issue controlled by design (e.g., limit on the sulfide, total sulfur and organic content)

Table 2-2. SKB Analysis of Buffer Significance in Terms of Depth of Damage by Corrosion in 1 Million Years (Based on 47-mm Thick Copper Waste Package)

Process	Comment	Damage Depth (mm)
Gamma radiation–air	Gamma radiolysis of nitrogen (initial + present in buffer) forms nitric acid. Unsaturated phase—amount of nitric acid corresponds to a film of a few nanometers in thickness.	8×10^{-6}
Radiolysis of water	Oxidant and hydrogen formed by radiolysis of water near the waste package. Gamma dose rate decreases substantially in the first 300 yrs.	0.0105
Atmospheric corrosion	Preclosure period.	0.001
Corrosion due to remaining oxygen	Oxygen initially present in the buffer, with reducing chemical conditions expected in the long-term	0.5
	Estimate based on more detailed considerations	0.102
Sulfide corrosion due to pyrite in the buffer	Pyrite initially present in the buffer surrounding the waste package. Extent of damage by chemical reaction of copper with sulfide: 0.1 mm and 0.9 mm for two types of bentonite material (MX80 and Ibeco-RWC). Upper bound estimates of damage: 0.4 mm and 2.9 mm, respectively.	0.4–2.9
	Pessimistic limit of the extent of damage. More detailed computations indicate 1-micron depth of damage if gradual pyrite dissolution and sulfide diffusion are considered. The extent of pyrite depletion in the buffer extends only 2 cm from the waste package. Pyrite from the backfill is considered unlikely to reach the waste package.	0.114
Sulfide corrosion due to microbes (organics existing in the buffer)	The largest amounts of organics are in the buffer and backfill, and closely attached to the clay minerals. Sulfate-reducing bacteria in commercial bentonite can become active after exposure to high temperature and salinity. The maximum sulfide availability is approximately 13,600 moles per waste package. This maximum can be constrained by design (e.g., selection of buffer material with lower sulfate content). The majority of sulfide potentially produced by microbes would not be available to dissolve in the groundwater. If dissolved, there would be limited diffusive transport of dissolved organics or any produced sulfide. During the unsaturated period, the corrosion rate would be low due to the low microbial activity under low humidity and elevated temperatures.	2 (top of the waste package)
Sulfide corrosion due to microbes (organics from other sources)	The estimates exclude sulfide originating by microbial action in the buffer and backfill. Other potential sources correspond to approximately 35 moles of sulfide per waste package. Organics in the buffer are approximately 20 percent of the organics in the backfill.	0.04

Table 2-2. SKB Analysis of Buffer Significance in Terms of Depth of Damage by Corrosion in 1 Million Years (Based on 47-mm Thick Copper Waste Package)

Process	Comment	Damage Depth (mm)
Sulfide corrosion due to microbes (balance hydrogen produced by corrosion of iron and steel)	Anaerobic corrosion of rock bolts and iron compounds remaining in the repository would produce hydrogen gas that could eventually produce sulfide via acetogens and sulfate-reducing bacteria. Mass balance estimates indicate a maximum sulfide production of 353 moles per waste package. The SKB calculation assumed immediate availability of sulfide at the waste package surface.	0.4
Sulfide corrosion due to sulfide in groundwater (intact buffer)	The sulfide transport rate limits the corrosion rate. The SKB calculation assumed that sulfide reacts with the entire surface of the copper outer shell, with a stoichiometric factor of 2 for the complete reaction between copper and hydrogen sulfide ($2Cu + HS^- + H^+ \rightarrow Cu_2S + H_2$).	0.7

Sources:
SKB. "Corrosion Calculations Report for the Safety Assessment SR-Site." Technical Report TR–10–66. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Co. December 2010a (Chapter 5 and references cited therein).

Table 2-3. Selected Near-Field Release Estimates and Significance of the Buffer From SKB Performance Assessments						
Case [Volume 3 of SKB (2011)]		Number of Waste Package Failed	Buffer Status	Near-Field Comparable Dose Equivalent (μSv/y)	Normalized Dose Equivalent§	Comments
1	Advection in a few boreholes (base case)*	0.12	Some failed	0.59	—	First waste package failure occurs at 50,000 yr.
2	Advection in all boreholes at start	0.17	All Failed	1	—	Groundwater flow and sulfide concentration insufficient to fail most waste packages.
3	Pinhole in waste package at start	1 (assumed)	Intact	3.7	—	Release to buffer at 1,000 yr. Waste package is assumed not to offer any flow resistance after 10,000 yr.
3a	Lost swelling pressure at tunnel crown	1 (assumed)	Intact	9.5	—	Implications for horizontal emplacement.
4a	Waste package failure due to shear-load	Failure time distribution: $10^3 – 10^6$ yr 0.079 waste packages failed	Thickness reduced by 10 cm	0.15	—	Waste package failure occurs when fractures in the rock are displaced more than 5 cm by seismic events, shearing the waste package.
4b	Waste package failure due to shear-load + buffer advection			0.34	—	
5a	Large hole in waste package at start	All	Intact	3,000	1	Release to buffer at 100 yr.
5b	Large hole in waste package at start + advection in a few boreholes	All	Failed (in a few boreholes)	400,000	~133†	Release to buffer at 100 yr. Peak release occurs at 100 yr.

Table 2-3. Selected Near-Field Release Estimates and Significance of the Buffer From SKB Performance Assessments

Case [Volume 3 of SKB (2011)]		Number of Waste Package Failed	Buffer Status	Near-Field Comparable Dose Equivalent (μSv/y)	Normalized Dose Equivalent[§]	Comments
5c	Large hole in waste package at start + fast spent nuclear fuel dissolution	All	Intact	1,000,000	~333[†]	Release to buffer at 100 yr.

Sources:
SKB. "Long-Term Safety for the Final Repository for Spent Nuclear Fuel at Forsmark: Main Report of the SR-Site project." Technical Report TR–11–01. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Co. March 2011.

Notes:
*This is one of several cases considered by SKB as a base case.
§Normalization added from a post-analysis of the SKB results for Cases 5a–5c.
†Normalized relative to Case 5a. 400,000/3,000 = 133.33; 1,000,000/3,000 = 333.33

3 SCENARIO ASSUMPTIONS

The purpose of these discussions was to examine the implicit assumptions in the current SOAR code, pertaining to buffer performance. Using the questions listed in Section 2 as a framework, aspects of the repository engineered barrier system and near-field environment considered relevant to buffer performance were discussed. The following sections highlight the consensus reached and decisions made on buffer conceptualization for potential abstraction in SOAR.

3.1 Initial Conditions

Discussions began by considering the point in the repository timeline when the initial state of the buffer should be defined. The SOAR code currently starts at repository closure (i.e., after all waste packages have been emplaced and the deposition holes and shafts sealed). Discussions considered the option of including the repository operations period to account for heterogeneities in emplacement across the repository footprint. Inclusion of the excavation damaged zone (EDZ) as part of the repository near-field also was discussed. For the nominal performance assessment scenario, it was decided to (i) retain the current approach in SOAR by initializing the model at the time of repository closure and (ii) assume a single representative waste package surrounded by the buffer, borehole, and EDZ with uniform properties. The EDZ could also be approximated by modifying the parameters for the first leg of the Far Field model component in SOAR. Heterogeneity may be considered as a possible variation to the nominal scenario.

3.2 Geologic Media

Host rocks discussed included salt, crystalline rock, clay, and other sedimentary rock. It was suggested to identify optional geologic media by their specific names (e.g., clay, alluvium, granite, etc.). The consensus was to retain the generic names currently used in the SOAR code (i.e., unconsolidated sediments, fractured rock, and porous rock); however, the SOAR development team needs to reassess the capability to model diffusive transport in clay host rock using the current GoldSim® pipe element. Also, the code may be restructured and parameterized to model faster flow and transport through the EDZ.

3.3 Waste Package Material

The main issue for waste package materials was the impact of flow and chemical composition of water potentially contacting the waste package on corrosion rates. Gas migration also was discussed with reference to small-scale laboratory and large-scale field experiments carried out by European organizations. Transport rates for hydrogen sulfide may be correlated to copper corrosion rates; however, it seems difficult to determine a direct relation of chloride concentrations to corrosion rates. Instead, the most feasible approach for performance assessment might be to sample from corrosion rate distributions that account for the presence of chloride. Regarding gas migration, small-scale laboratory experiments conducted under the Fate of Repository Gases (FORGE)[2] program suggest that gas migration occurs through dilational pathways in the rock; however, the metrics defining travel time and breakthrough conditions are difficult to determine (Graham and Harrington, 2014). Furthermore, larger scale field experiments conducted at the Äspö Hard Rock Laboratory in Sweden do not suggest a consistent pattern of gas migration (Cuss, et al., 2010).

[2]<https://www.bgs.ac.uk/forge/> (30 June 2015)

Participants discussed the possibility of waste package damage by corrosion in tens of thousands of years if advection dominates flow through the buffer. This discussion lead to the concept of time-dependent loss of buffer mass, as a possible abstraction for buffer erosion due to fluid forces. In addition, the SOAR development team was asked to consider including additional chemical constituents in the GoldSim species configuration. In the case of sulfide, the option of using offline calculations to compute corrosion rate as a function of hydrogen sulfide concentrations was discussed.

3.4 Thermal Model

The discussion focused on whether to consider elevated temperatures (i.e., above 100 °C) in the performance assessment of the repository near field. One option considered was to set the low temperature mode (i.e., less than 100 °C) as the nominal scenario and the high temperature mode as an alternative. It was noted that DOE is currently studying the high temperature mode, including the use of a sacrificial buffer to account for buffer degradation and failure. Because of uncertainties in the current knowledge base, it was decided not to implement a high-temperature scenario in the performance assessment model until the coupled processes and corrosion teams have conducted additional literature reviews. Concurrently, the SOAR development team would contemplate potential abstractions to represent temperature-dependence of waste form dissolution rates, waste package corrosion rates, chemical stability of radionuclide-bearing phases and solubility limits, chemical stability of buffer materials, sorption parameters, and diffusion coefficients.

3.5 Modeled Buffer Functions

Participants discussed ways to split radionuclide releases among advective and diffusive transport pathways in the buffer. The default case in SOAR assumes radionuclide release and transport occurs only by diffusion through an intact buffer. Additional rules are implemented for allowing advective releases, depending on whether the buffer is degraded or absent. The SOAR team suggested exploring alternative abstractions through SOAR experiments and possible modification of the existing buffer degradation module.

4 PROCESSES INFLUENCING BUFFER PERFORMANCE

The objectives of these discussions were to (i) further examine the significance of processes associated with the buffer to overall repository system performance and (ii) identify metrics to quantify the degree to which the buffer can provide its designated barrier capabilities. Based on the processes listed in Table 2-1, participants classified each process as either significant (S) or insignificant (N) to the performance of the repository. Table 4-1 shows the assignments defined for each of the processes listed.

The performance metrics available in the current version of SOAR include flow rate, corrosion rate, time of failure, waste package breach area, number or fraction of failed waste packages, and sorption parameters. Additional metrics could be defined for the buffer in terms of degree of saturation and colloid-facilitated transport. However, because of uncertainties in the scientific knowledge base, the workshop participants were unable to reach a consensus on relationships between the buffer environmental conditions (e.g., temperature, water chemistry, and buffer mineralogy) and processes needed to inform potential buffer performance metrics.

After further discussions, the following five concepts associated with buffer evolution and performance were identified as high-priority areas for potential inclusion in the next version of

Table 4-1. Classification of Processes Associated With Buffer Performance			
Process	**S/N**	**Process**	**S/N**
Heat transport	S	Transport of radionuclides by a gas phase	S
Freezing	N	Diffusive transport of species that control corrosion rate and radionuclide transport	S
Water uptake and transport in unsaturated conditions	S	Alteration of impurities	N
Water transport under saturated conditions	S	Aqueous speciation and reactions	N
Gas transport/dissolution	S	Radiation-induced transformations	N
Piping/erosion	S	Radiation attenuation/heat generation	N
Colloid transport	N	Liquefaction	N
Swelling/mass redistribution	S	Radiolysis of pore water	N
Advective transport of species	S	Material composition	S
Montmorillonite transformation	S	Iron-bentonite interaction	S
Montmorillonite colloid release	N	Osmosis	N
Microbial processes	N	Waste-clay interaction	S
Cementation	N	Mechanical alteration of clay by gas breakthrough	—
Sorption (including ion exchange)	S	Speciation of radionuclides	N

the SOAR code: (i) changes in mineralogy, (ii) two-phase flow and transport, (iii) advective flow and transport through preferential pathways and existing conduits, (iv) piping and erosion due to fluid flow, and (v) gas breakthrough at the host rock interface.

5 MODEL ABSTRACTIONS AND RESIDUAL UNCERTAINTIES

The goals of the discussions in this session were to consolidate the decisions from the previous two sessions and initiate the development of a nominal performance assessment scenario that incorporates the evolution of an engineered buffer. First, the main elements of the nominal scenario were defined, followed by a discussion of potential ways to abstract these elements into the SOAR performance assessment model. Lastly, residual uncertainties were identified for further literature surveys and research by the coupled processes, corrosion, and SOAR development teams. The following sections summarize concrete ideas on how different components of the system would be modeled in SOAR.

5.1 Elements of the Nominal Scenario

As discussed in Section 3, the nominal or reference scenario for buffer performance assessment modeling will be developed assuming a low temperature (i.e., less than 100 °C) operating mode. The current version of SOAR does not include any temperature-dependent model. Significant uncertainties remain about how changes in temperature during the lifetime of the repository would affect the condition of the buffer and the dynamics of processes controlling the behavior of the buffer. Temperature-dependent conditions, such as degree of water saturation, mineral composition, and water chemistry, are not well characterized. Likewise, flow rates, waste package corrosion rates, radionuclide solubility, and sorption rates must be related to temperature in order to develop reasonable abstractions to support performance assessments of elevated-temperature systems. The coupled processes, corrosion, and performance assessment teams recognized the potential need to explore the technical literature, as well as DOE and international programs reports, for insights to guide abstraction of temperature-dependence into the SOAR input parameters and simplified models.

An important aspect of buffer abstraction is the incidence of piping and erosion of buffer material under advective flow conditions. This subject was considered as part of the SKB performance assessment, but was excluded due to low likelihood. Previous experiments have been carried out with the SOAR code to examine the relative dominance of advective versus diffusive transport between the waste packages and the host rock. These experiments were conducted as part of collaboration between NRC and CNWRA to develop a risk insight methodology associated with the back end of the nuclear fuel cycle (Osidele, et al., 2012). The rate of transport of potentially corrosive agents (e.g., hydrogen sulfide in the case of copper waste packages) from the host rock and the transport of radionuclides released from the waste package depend on the integrity of the buffer. An intact or fully sealed buffer will limit diffusive transport in both directions. Faster release rates might occur if advective pathways develop due to erosion damage to the buffer and intercepting fast flow paths, such as water conducting fractures and faults. The SOAR code currently includes a buffer degradation module that can be enhanced with additional knowledge and abstraction of processes that may affect the mechanical integrity of the buffer material.

Gas buildup and migration were considered for potential inclusion in the nominal scenario. Due to unresolved uncertainties regarding the detrimental or beneficial impacts to the repository system performance, a decision could not be reached on the relevance of gas buildup and transport. The significance of gas (including hydrogen) generation from corrosion processes and the potential for gas migration to affect the mechanical integrity of the buffer should be informed by available analyses in the literature, to decide whether related scenarios and abstractions are needed in the SOAR code. The implications of gas generation and potential two-phase flow also should be considered.

Additional components of the nominal scenario were discussed, including early waste package failures, disruptive events, and climate changes. Early waste package failure provides a means for radionuclide release during the thermal period when the buffer is partially saturated and not fully sealed. Although the SOAR code can be readily modified using GoldSim source term elements to account for early waste package failure, the environmental conditions in the buffer during the thermal period (e.g., temperature profile, buffer mineralogy, and effects on transport properties) have yet to be adequately conceptualized for any needed abstraction. Waste package failure under disruptive events can be implemented in SOAR; however, additional process knowledge is needed to understand and specify the condition and performance of the buffer under such events. Regarding climate change, uncertainty remains about the impacts of potential future climate change on flow rates and water chemistries. In addition, the potential impacts of climate change would depend on the repository design and site-specific features of the repository location. Because of the difficulty of evaluating site-specific questions on the basis of a generic performance assessment code, such as SOAR, it was decided not to consider issues pertaining to climate change in the reference scenario.

5.2 Residual Uncertainties

Temperature profiles and functional representations of the relationships between temperature and various waste package and buffer processes have yet to be determined. The discussions recognized these relationships may be complicated by dependence on multiple interacting factors. For example, while SOAR currently simulates waste package corrosion and transport using corrosion rates, solubilities, diffusion coefficients, and sorption coefficients, the temperature-dependence of these parameters might be influenced by the dynamic changes in intermediate properties, such as buffer mineralogy, water chemistry, saturation, porosity, and several other buffer environmental conditions. Such complex relationships may require more than a simplified response function expression to capture temperature- and time-dependence. The GoldSim software provides several tools, including sampling distributions and multidimensional lookup tables to facilitate complex abstractions.

The potential process complexities described in the previous paragraph also increase the likelihood that counteracting processes may exist, thereby limiting the potential consequences of a given process. For example, as discussed in Section 2.1, gas buildup and migration could be both detrimental and beneficial to repository system performance. On one hand, if gas buildup is not dissipated fast enough, the ensuing pressure may compromise the buffer and the waste package. On the other hand, the absence of pathways for fast relief of gas pressures also could contribute positively to the barrier capability of the buffer to limit radionuclide transport. Abstractions for such situations would require extensive understanding of the relevant process interactions.

6 CNWRA SUGGESTIONS FOR FUTURE WORK ON THE SOAR CODE

The SOAR model is intended to support NRC with a flexible scoping tool for obtaining timely risk and performance insights for various potential high-level waste disposal options. By design, the abstractions included in the SOAR code are intended to be relatively simple or generic representations of repository features, events, and processes. The purpose is to retain flexibility, efficiency, and transparency of the code, and to facilitate interpretation of results and identification of limitations. The SOAR code might not be able to fully capture complex mechanisms without extensive structural modifications. For example, a model structure with a more process-oriented underpinning (i.e., accounting for detailed physical processes and couplings) could be incorporated through a GoldSim dynamically linked library (DLL). Application to cases such as engineered buffers in geologic repository systems presents uncertainties that may be resolved only when site-specific characteristics are accounted for. However, attaining such level of detail and specificity is not the goal of SOAR.

The discussions described in Section 5 highlight uncertainties challenging the development of a complete abstraction of buffer processes for a reference or nominal performance assessment scenario. Further examination of the scientific and technical literature is needed to reduce these uncertainties and develop a knowledge base to support future work on the SOAR code. Once the required knowledge base becomes available, conceptualizations for buffer behavior and interactions with other repository near-field components can be developed for abstraction into the SOAR code. In the meantime, computational experiments can be designed to test time-dependent process abstractions, using the broad selection of tools and functions available in the existing SOAR model. For example, the current version of SOAR includes a simple demonstration of a way to incorporate time-dependent corrosion rates. A similar approach can be adopted to account for temperature dependence using hypothetical temperature evolutions and system response.

To simplify the conceptualization of buffer performance and subsequent abstraction of processes in SOAR, it is desirable to analyze and classify multiple near-field radionuclide transport cases, using a generic framework without reference to specific rock structures. The goal of this analysis would be to develop a comprehensive classification of radionuclide transport scenarios that are common to several repository designs and host rock types. Insights from the discussion sessions indicate a variety of scenarios would be restricted to diffusive transport through the buffer, even for situations where the buffer is partially sealed. CNWRA staff proposes modeling a few test cases, using variable diffusion coefficients to account for the state of the buffer (i.e., fully or partially sealed). Examples of suggested transport pathways include (i) vertical diffusion discharging to the water table and (ii) diffusion to intercept a major water conducting feature. Results of these tests would be presented using stylized flow diagrams and also compiled in simple spreadsheet formats.

Activities to support SOAR development could include interacting with the coupled processes and corrosion teams through follow-on model integration experiments and technical workshops. Approaches can be explored to (i) simulate unsaturated buffer and the effects on waste package corrosion and early radionuclide release; (ii) account for dynamic buffer resaturation and sealing of gaps, and the effects on waste package corrosion and radionuclide release; and (iii) develop models or abstractions for buffer erosion and its effect on waste package lifetime. Independent analyses can be performed on specific processes to evaluate whether they merit explicit consideration for abstraction into SOAR. Examples of subjects for such analyses may include:

- Heterogeneous resaturation within the buffer material surrounding a single waste package
- Development of a damaged zone in the clay material
- Consequences of large-scale heterogeneity on the state of the buffer throughout the repository
- Selection of a representative system (e.g., waste form/waste package/buffer) that properly represents the variability in the system
- Hydrogen buildup and its effect on waste package lifetime (e.g., hydrogen embrittlement of carbon steel combined with residual stresses in welded zones, uneven stresses on the waste package evolving with time, and enhanced susceptibility to failure due to seismic events)
- Effect of hydrogen buildup on waste form dissolution and radionuclide transport
- Dominant effects of elevated-temperature systems

This list of subjects is not intended to be comprehensive; it is intended only to delineate areas of potential work related to further development of the SOAR code.

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APPENDIX A

2015 NRC-CNWRA BUFFER CONCEPTUALIZATION WORKSHOP AGENDA

Agenda

2015 NRC-CNWRA Buffer Conceptualization Workshop

February 24, 2015

9:00 AM to 5:00 PM ET
Location: HQ–3WFN–13A28–29p at NRC; A237 at CNWRA (via Video Conferencing)

Time in ET

9:00	Introduction	Gwo Osidele
9:10	Summary of State of Knowledge and Key Gaps	Fedors, Manepally Mohanty Ahn, He, Shukla
10:10	Break	
10:20	Scenario Assumptions	Facilitator: Pensado
	Initial State(s) of the Buffer	
	Functions of the Buffer	
12:00	Lunch	
1:00	Key Processes Influencing Buffer Performance	Facilitator: Markley
	Buffer Performance Metrics	
2:30	Break	
2:40	Buffer Evolution and Scenarios	Facilitator: Gwo
	Summary of Model Abstractions and Residual Uncertainties	
4:30	Conclusions	Osidele Gwo

APPENDIX B

2015 NRC-CNWRA BUFFER CONCEPTUALIZATION WORKSHOP DISCUSSION TOPICS

Discussion Topics for the
2015 NRC-CNWRA Buffer Conceptualization Workshop

February 24, 2015

1. Introduction

2. Summary of State of Knowledge and Key Gaps
    - *Brief presentations on current understanding of processes affecting buffer and waste package performance. The purpose is to provide preliminary insights to support the discussion topics (item #s 3–9) below.*
        - *Evolution of environmental conditions in the buffer*
        - *PA perspective on state of knowledge of key issues related to buffer*
        - *Waste package materials*

3. Scenario Assumptions
    - *Host rock type and properties (e.g., water chemistry)*
    - *Canister material*
    - *Buffer material composition and water chemistry*
    - *Thermal operating mode (temperature profile)*
    - *Climate change and disruptive events*

4. Initial State(s) of the Buffer
    - *Describe initial states on the basis of scenario assumptions in item #3*

5. Functions of the Buffer
    - *Containment (restrict flow around canisters; isolate waste from biosphere)*
        - *low hydraulic conductivity supports dominance of diffusive flow*
        - *swelling pressure high enough for buffer to self-seal (montmorillonite content)*
        - *limit microbial activity on the waste package surface (limit sulfur content)*
    - *Retardation (prevent or reduce radionuclide transport to biosphere)*
        - *low hydraulic conductivity*
        - *radionuclide sorption on buffer minerals*
        - *filter colloidal particles*
    - *Mechanical Stability*

6. Key Processes Influencing Buffer Performance
    - *Classify processes under the three primary buffer functions*
    - *Discuss the timeframes in which each process is relevant*

7. Buffer Performance Metrics
    - *Identify quantifiable indicators of the degree to which the buffer can provide its designated safety functions (for example, in terms of saturation, flow rate, corrosion rate, time of failure, waste package breach area, number or fraction of failed waste packages, sorption, colloid-facilitated transport, etc.)*

8. Buffer Evolution and Scenarios
    - *Main (or nominal) scenario (expected evolution)*
    - *Less probable scenarios (loss of safety functions)*

9. Summary of PA Model Abstractions and Residual Uncertainties

10. Conclusions