Strål säkerhets myndigheten
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Technical Note

2012:29

Initial review of chemical and erosional processes within the buffer and backfill – Geochemical processes

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SSM perspektiv

Bakgrund

Strålsäkerhetsmyndigheten (SSM) granskar Svensk Kärnbränslehantering AB:s (SKB) ansökningar enligt lagen (1984:3) om kärnteknisk verksamhet om uppförande, innehav och drift av ett slutförvar för använt kärnbränsle och av en inkapslingsanläggning. Som en del i granskningen ger SSM konsulter uppdrag för att inhämta information i avgränsade frågor. I SSM:s Technical note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Denna rapport består av en ”Technical Note” inom SSM:s inledande granskning av SKB:s säkerhetsredovisning SR-Site. Syftet med denna inledande granskning av frågorna kring geokemiska processer i buffert och återfyllnad i slutförvarsanläggningen är att få en bred granskning och belysning av SR-Site och underreferenser samt att identifiera eventuella behov av kompletterande information eller förtydliganden som SKB bör tillfoga ansökansunderlaget.

Författarnas sammanfattning

De dokument i SR-Site som är relevanta till detta granskningsområde bedöms vara generellt i tillräckligt hög kvalitet för att utgöra underlagsmaterial för vidare granskning i huvudgranskningsfasen av SSM:s GLS- (granskning av långsiktig säkerhet) projekt. Behov av kompletterande information eller förtydliganden har dock identifierats inom flera specifika ämnen (Appendix 2). Några specifika granskningsfrågor har också rekommenderats till fördjupade granskning i huvudgranskningsfasen (Appendix 3).

Projektinformation

Kontaktperson på SSM: Jinsong Liu
Diarienummer ramavtal: SSM2010-4230
Diarienummer avrop: SSM2011-4204
Aktivitetsnummer: 3030007-4004

SSM perspective

Background

The Swedish Radiation Safety Authority (SSM) reviews the Swedish Nuclear Fuel Company's (SKB) applications under the Act on Nuclear Activities (SFS 1984:3) for the construction and operation of a repository for spent nuclear fuel and for an encapsulation facility. As part of the review, SSM commissions consultants to carry out work in order to obtain information on specific issues. The results from the consultants' tasks are reported in SSM's Technical Note series.

Objectives of the project

This report consists of a Technical Note in SSM's initial review phase of SKB's safety analysis SR-Site. The aim of the initial review of issues concerning geochemical processes in buffer and backfill in a final repository is to make a broad illustration and review of SR-Site together with its subordinate references, as well as to identify potential needs for complementary information or clarification which SKB should supplement to its license applications.

Summary by the authors

The SR-Site documentation relevant to this review topic was found to be of sufficiently high quality overall to justify further consideration in the Main Review Phase of SSM's PCS (Post-closure safety) project. Several specific topics for which complementary information and clarifications should be requested from SKB were also identified (Appendix 2). Specific review topics for consideration during the Main Review Phase are recommended in Appendix 3.

Project information

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Technical Note 10

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Initial review of chemical and erosional processes within the buffer and backfill – Geochemical processes

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Contents

1. Introduction

This report summarizes the results of a preliminary review of various aspects of SKB's safety assessment SR-Site dealing with geochemical processes within the buffer and backfill in a KBS-3 repository at Forsmark. The objective of the review was to determine whether the documentation in SR-Site and supporting references is reasonably complete and of sufficiently high quality to justify a more detailed review of geochemical processes that could affect the safety functions of the buffer and backfill, and in particular to identify any complementary information and clarifications needed from SKB before such a review could be carried out.

The main focus of the present review, which is part of the Initial Review Phase of SSM's Post-Closure Safety (PCS/GLS) project (Dverstorp et al., 2011), concerned specifically SKB's reporting of processes related to the geochemical evolution of the bentonite buffer in deposition holes and within backfill materials in deposition tunnels. This entailed consideration of fundamental geochemical processes, including ion-exchange, illitisation and other clay-mineral hydrolysis reactions, reactions of bentonite minerals with hyperalkaline fluids, dissolution/precipitation of accessory minerals, interactions with corrosion products, and other related processes described in SKB reports. Colloid chemical processes related to chemical erosion of the buffer and backfill, and chemical/geochemical processes affecting the speciation, solubility and sorption behaviour of radionuclides, were excluded from this review assignment, however. Appendix A provides a listing of SKB reports considered in the review. Full bibliographic details are provided in Section 4.

2. Main Review Findings

A number of topics related to the geochemistry and geochemical evolution of buffer and backfill materials were considered in the review. These topics included:

- Completeness of the safety assessment;
- Scientific soundness and quality of the SR-Site safety case;
- Adequacy of relevant models, data and safety functions;
- Handling of uncertainties;
- Preliminary assessment of safety significance; and
- Quality, in terms of transparency and traceability, of information in SR-Site and associated references
- Feasibility of manufacturing, construction, testing, implementation, and operation of buffer and backfill materials.

Review findings are described below for each of these topics.

2.1. Completeness of the safety assessment

The question whether SR-Site is complete in its treatment of geochemical processes within the buffer and backfill was taken to concern whether there are any obviously missing pieces of information needed to carry out a more detailed review. If appropriate, such a review would be conducted during the Main Review Phase of SSM's PCS project (Dverstorp et al., 2011). SR-Site is considered to be sufficiently complete in this sense, but the following topics may need further clarification and more detailed review during the Main Review Phase.

2.1.1. Material properties

Discussions in SR-Site concerning safety functions, compositions, initial states, impacting processes and selection of materials are summarized in Sections 5.5, 7.4.3, 8.3.2, and 8.4.3 for the buffer, and in Sections 5.6, 7.4.4, 8.3.3 and 8.4.4 for the backfill (SKB, 2011). Much of the supporting information to these summaries is provided in the production reports referenced. Although this information is considered to be adequately complete, SKB should be requested to provide additional clarification concerning the following topics (Appendix 2):

Commercial suppliers of the two different bentonite types considered for use as buffer materials (SKB 2011; page 180) could use dissimilar processing techniques or refinements to produce their 'as-delivered' material. Documentation addressing whether such differences, if any, could directly or indirectly result in any adverse impacts on safety functions should be provided.

Although the exchange-site compositions of montmorillonites in MX-80 and Ibeco RWC bentonites differ significantly (SKB 2011; Table 5-10), these differences do not appear to have any significant impact on swelling pressure (SKB 2011; Figure 5-14). SKB should provide similar documentation addressing whether such differences could significantly impact other safety-relevant properties of the two bentonites (e.g., susceptibility to chemical erosion). SKB should also provide documentation on expected, as well as plausible, ranges in the Fe(III)/Fe(II) contents of montmorillonites in MX-80 and Ibeco RWC bentonites.

2.1.2. Treatment of extraneous materials

Sections 10.3.11 and 10.3.12 of SR-Site (SKB 2011) briefly consider the effects of organics, high-pH inducing cements and iron on the evolution of near-field chemical conditions as well as chemical conditions in the cement region under the copper bottom plate, respectively. Because both high-pH conditions and the presence of metallic iron could have the potential to impact the "buffer transformation" scenario, the question arises as to why SR-Site did not consider 'buffer transformation' in an illustrative scenario (Section 13.7). SKB should therefore be requested to clarify why "partial buffer transformation attributable to extraneous materials" was not considered as a 'less probable' scenario to be calculated and included in the overall risk summation (Appendix 2).

2.1.3. Retardation safety functions

In certain scenarios, including those involving canister failure due to 1) a shear load, 2) an isostatic load, or 3) a growing pinhole failure, the buffer and backfill are assumed to remain intact (though possibly with altered dimensions) and to retain their retardation properties (SKB 2011; Sections 13.6 and 13.7). The effects on these properties of geochemical processes occurring within the buffer and backfill in response to environmental conditions set up by corrosion of the Cu container and iron insert are apparently not considered in SR-Site, however. Such processes could, for example, lead to partial or complete alteration of primary montmorillonite to less swelling or non-swelling Fe-bearing phases having a lower sorption capacity for radionuclides released from spent fuel. Strongly reducing conditions resulting from corrosion of the iron insert could also reduce any Fe(III) occupying octahedral sites in montmorillonite, thereby potentially leading to alterations in physical properties of the buffer and backfill (e.g., Stucki, 2011). SKB should be requested to provide clarification as to whether geochemical processes that could potentially affect retardation properties of the buffer and backfill in certain canister failure scenarios should be considered as 'less probable' scenarios to be calculated and included in the overall risk summation (Appendix 2).

2.1.4. Consistency of assumptions in geochemical models

During nearly 30 years of research and development SKB has evaluated and used a number of different geochemical models to interpret and predict various aspects of the chemistry and chemical evolution of buffer and backfill materials. Three such approaches include, for example:

- an osmotic model to explain clay swelling behaviour;
- ion-exchange and surface-complexation models to describe the long-term chemical evolution of pore fluids; and
- empirical expressions describing the kinetics of montmorillonite illitization.

The assumptions underpinning such different modelling approaches are not always mutually consistent. For example, ion-exchange models assume that the compositions of octahedral and tetrahedral sites in the smectite framework are fixed. In contrast, models for the illitization of smectite assume variable tetrahedral charge arising from the isomorphous substitution of Al^{3+} for Si^{4+}. These two different assumptions are fundamentally inconsistent, but the models are nevertheless separately applicable under certain conditions. For example, ion-exchange models are valid as long as the extent of any tetrahedral substitutions is sufficiently small that the framework composition remains effectively unchanged.

SKB should be requested to provide clarification concerning the consistency of assumptions used in the various geochemical models supporting SR-Site (Appendix 2). This should include a description of all such models, identification of assumptions used in the models, a systematic analysis of inconsistencies among these assumptions, and identification of conditions for which any such inconsistencies can be considered unimportant.

2.2. Scientific soundness and quality of SR-Site

The adequacy of the scientific basis underpinning the treatment of buffer/backfill geochemical processes in SR-Site was evaluated with the following questions in mind:

- Are key scientific conclusions adequately supported and justified, and
- Are necessary references provided and are they sufficiently specific?

Issues concerning the first of these questions are discussed in the following subsections. All references reviewed in this review assignment were found to be sufficiently specific.

2.2.1. pH dependence of smectite stability

Smectite clays in the buffer and backfill could become unstable, converting into illite or various zeolites, for example, if these barriers were to come into contact with high-pH leachates resulting from the interaction of various cementitious materials in the repository with groundwater. For this reason a safety function indicator criterion, pH < 11, has been adopted in SR-Site for the geosphere safety function R1 (provide chemically favourable conditions) related to both containment and retardation (SKB 2011; Sections 8.3 and 8.4, respectively). In this context "stability" relates only to the ability of smectite to resist transformation to an unspecified non-smectite phase, i.e., it does not preclude possible changes in the chemical composition of smectite solid solutions.

The scientific basis in selecting this pH criterion rests on a set of arguments that seem only marginally relevant to the question of smectite stability (SKB 2011; Section 10.3.10). One line of reasoning is that the solubility of quartz is known to increase with increasing pH when pH > 9 (SKB 2011; page 396). Why this observation is considered relevant to the issue of smectite stability is unclear. For example, although quartz (and smectite) solubilities may increase with increasing pH, this does not necessarily mean that quartz is thermodynamically unstable in high-pH solutions. Quartz would be stable in such solutions if dissolved silica concentrations correspond to the equilibrium solubility of quartz at the pressure and temperature of interest.

A similar line of reasoning is based on an experimental study of smectite dissolution kinetics between pH 7 and 14 at 25, 50 and 70^{o}C (Huertas et al., 2005). The experimental results indicate that surface-area normalized rate constants for smectite dissolution under far-from-equilibrium conditions tend to increase with increasing pH (Figure 2.2.1_1). Huertas et al. (2005) speculate that the rate at which the rate constant increases with increasing pH changes abruptly at about pH 11, although this view seems to be based on a rather subjective fit of estimated rate constants with their experimental counterparts. Based on these results, SKB concludes that smectite will be stable in the repository environment for at least 1,000,000 years as long as the pH of buffer/backfill porewaters remains below pH 11 (SKB 2011, page 397).

The technical basis for this conclusion may not be adequately supported for several reasons. The dissolution rate can only reflect how quickly smectite might achieve equilibrium with an aqueous solution at a given pH and temperature, not whether smectite would be thermodynamically stable under such conditions. The conclusion is moreover based on the pH-dependence of the dissolution rate constant at various temperatures, whereas the actual dissolution rate will also depend on smectite reactive-surface area, and thus on the microstructure of compacted buffer and backfill materials. The nature of such microstructure is uncertain and a subject of much debate (e.g., Savage et al., 2011), which suggests that interpretations of smectite stability based solely on the pH-dependence of the dissolution rate constant may be overly simplistic. Also, because smectites are multi-constituent solids, equilibrium stability relations cannot be interpreted based on pH alone. Such relations have been interpreted in terms of the aqueous activities and activity ratios of all constituents affecting the stability of smectite and possible alteration phases, including H^+ (e.g., Garrels, 1984; Aagaard and Helgeson, 1983). SKB has apparently chosen not to follow this approach for reasons that should be clarified.

Given the safety relevance of the pH < 11 safety function indicator criterion and the questionable justification for selecting this criterion in SR-Site, SSM should further evaluate the reasoning behind this justification during the Main Review Phase of the PCS project (Appendix 3). Such an evaluation should include a detailed review of established alternative methods to those considered by SKB for interpreting smectite stabilities as a function of temperature, mineral chemistry and aqueous solution chemistry.

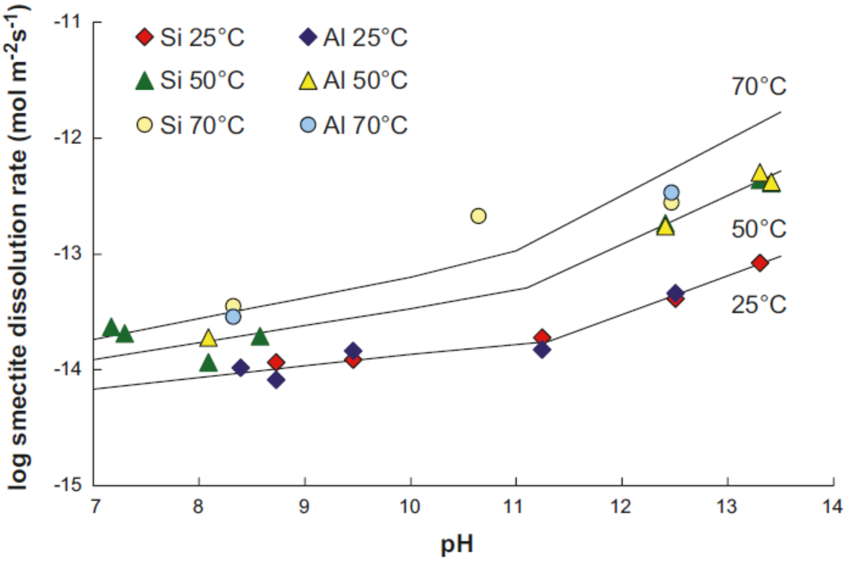

Figure 2.2.1_1. Experimental (symbols) and estimated (lines) surface-area normalized dissolution rates for a smectite (Huertas et al., 2005).

2.2.2. Geochemical models

Geochemical conditions in the buffer and backfill are expected to evolve during the early thermal period (up to several thousands of years in duration) and subsequent isothermal period of repository evolution. The evolving conditions will be controlled by complex, and possibly strongly coupled, THMCB processes that could result in substantial changes in the physical properties and associated safety function indicators of these barriers.

SR-Site includes a description of the expected chemical evolution of the repository host rock and near field during the reference glacial cycle (SKB 2011; Sections 10.3 and 10.4). The predicted chemical evolution of the buffer and backfill during this time is based primarily on the results of a geochemical modelling study (Sena et al., 2010), which builds upon earlier models (Arcos et al., 2006; 2008) and is claimed to adequately simulate the diffusion behaviour and changes in mineralogy observed in the LOT A2 parcel investigations (Karnland et al., 2009).

The Sena et al. (2010) model may be deficient in a number of respects. It does not consider the key component Al_2O_3, and consequently dissolution/precipitation reactions involving the dominant smectite clays and other alumino-silicates in buffer and backfill materials are unfortunately ignored. Smectites are instead treated in terms of a fictive ion-exchanger phase, which is assumed to have a fixed, though unspecified, composition. This assumption conflicts with findings from the LOT A2 investigations, which indicate that the CEC of smectites tends to increase at the highest temperatures (130^{o}C) within as little as 6 years due to an uptake of Mg in octahedral positions and a loss of Si from tetrahedral sites (Olsson and Karnland, 2011). Equilibrium is also assumed in the model because transport processes in the buffer/backfill are expected to be slow and because time scales considered in the model are long (Sena et al., 2010; page 14). This assumption may not be appropriate if the rates of diffusional solute transport are comparable to the rates of heterogeneous, mineral-hydrolysis reactions because the relevant reactive-transport processes would then be coupled and hence time dependent (Savage et al., 2011). In such a case more realistic models may be needed to account for the effects of buffer/backfill density-dependent microstructure on reactive mineral surface areas.

Because the Sena et al. (2010) model seems to be overly simplistic for the reasons stated above, model results used in SR-Site may not be adequately bounding with respect to the long-term chemical evolution of the buffer and backfill. Such deficiencies may be especially problematic for models of buffer/backfill chemical evolution during the thermal period because re-saturation times in relatively dry deposition holes at Forsmark could extend for as long as several thousands of years, thus potentially prolonging the exposure of the buffer to elevated temperatures and temperature gradients. SSM should therefore conduct a detailed review of SKB's SR-Site model of buffer/backfill chemical evolution. If necessary, the review should include the development of an independent modelling capability that can be used by SSM to evaluate alternative assumptions and conceptual models (Appendix 3).

2.2.3. Donnan equilibrium

Documentation supporting SR-Site contains conflicting views on the importance of the Donnan equilibrium in controlling the diffusion properties of buffer and backfill materials. One view holds that diffusion will be controlled both by ion exchange and by a Donnan equilibrium established between aqueous solutions occupying smectite interlayer spaces and an external solution (SKB, 2010d; Birgersson and Karnland, 2009). An opposing view maintains that in domains larger than those typically used in experimental through-diffusion cells, Donnan equilibria and anion exclusion are relatively unimportant and can be ignored in models of buffer/backfill geochemical evolution (Sena et al., 2010).

These contrasting views appear to be fundamentally incompatible. If so, this is an issue that is particularly safety-relevant because the Donnan equilibrium is invoked by SKB as an important diffusion-controlled constraint on the swelling pressure (SKB, 2011, Section 10.3.9; SKB, 2010d, Section 3.5.8) and because swelling pressure is an overarching direct or indirect safety function indicator for both the buffer and backfill. SKB should be requested to clarify their position on this issue (Appendix 2). Depending on SKB's clarification, a comprehensive, self-consistent re-evaluation of this issue may be needed during the Main Review Phase (Appendix 3).

2.3. Adequacy of relevant models, data and safety functions

The following questions were considered with regard to the adequacy of models, data and safety functions used in SR-Site, specifically as they pertain to geochemical processes affecting the buffer and backfill:

- Are key datasets and data treatments (e.g., derivation of effective parameters) used in the evaluations adequately described and referenced;

- Are mathematical models sound and adequately described; and

- Are relevant safety functions, safety function indicators, and safety function indicator criteria adequately explained and justified?

Comments addressing these questions are summarized below. All references to mathematical models considered in this review assignment were found to be adequately described, but access to these models, input files and supporting databases should generally be improved (Section 2.6.1). An issue concerning justification for the SR-Site pH < 11 safety function indicator criterion is discussed in Section 2.2.1.

2.3.1. Numerical geochemical models of buffer evolution

The geochemical evolution of the buffer is evaluated in SR-Site over two distinct time periods: an early thermal period lasting up to 2000 years (see SKB 2011; Section 10.3.8) and a later isothermal period (Sena et al., 2010). Two different numerical codes were used to evaluate conditions during these two periods: TOUGHREACT for the thermal period and PHAST for the isothermal period. The capabilities of these two codes are generally similar, but PHAST was used by Sena et al. (2010) to evaluate the effects of pH-buffering by clay minerals in terms of ion-exchange and surface protonation/deprotonation reactions (together with carbonate mineral dissolution/precipitation), whereas TOUGHREACT can only consider the effects of ion exchange. Also noteworthy is the fact that different thermodynamic databases were used to support simulations using these two codes [i.e., an “EQ3/6”-compatible database was used for the TOUGHREACT simulations whereas a database compatible with SKB’s Trac system (Duro et al., 2006) was used for the PHAST simulations (Sena et al., 2010)].

These differences in code capabilities and thermodynamic databases raise the question whether the respective modelling results are sufficiently consistent that the evolutionary transition from the thermal period to isothermal period can be considered as effectively seamless. Such consistency could be evidenced, for example, if the effects on pH-evolution of surface protonation/deprotonation reactions considered in the PHAST model were found to be insignificant compared to the effects of ion exchange. To independently evaluate this question, however, would require that SSM have access to the respective numerical models, all relevant input files, and thermodynamic databases used by Sena et al. (2010). It is therefore recommended that SSM should request such access from SKB (see Section 2.6.1 of the present report).

2.4. Handling of uncertainties

This review topic concerns whether all known and relevant uncertainties related to geochemical processes within the buffer/backfill have been identified, analysed and discussed in sufficient detail. Results of the present review assignment indicated that such detail is adequate, with exceptions discussed in the following subsections.

2.4.1. Extraneous materials

Interactions involving the buffer/backfill and extraneous, or “stray”, materials are generally ignored in SR-Site because it is considered unlikely that such materials would be deliberately, or inadvertently, emplaced directly within these barriers (SKB 2010c). Stray materials in other parts of the repository could react with the local geochemical environment or serve as food-sources for microbiological activity, however, possibly resulting in significant transient changes in the chemistry of groundwaters that could subsequently interact with the buffer/backfill (Hallbeck, 2010). SSM should consider whether significant transformation of the mineralogy and physical properties of buffer/backfill materials due to such indirect impacts from extraneous materials is possible, and, if so, whether such impacts should be considered as a less probable scenario that should be evaluated and included in the SR-Site overall risk summation (Appendix 3).

2.4.2. Buffer and backfill microstructure

The geochemical evolution of the buffer and backfill may be influenced by microstructural constraints on the porosity of these materials because the porosity influences such properties as ion diffusivities and reactive mineral surface areas (e.g., Apted et al., 2010; Savage et al., 2011). Whether these barriers consist of different porosity types, or of a single type of porosity, is currently a matter of on-going international debate (e.g., Birgersson and Karnland, 2009; Tournassot and Appelo, 2011; Hedström and Karnland, 2012). The uncertain nature of porosity types in compacted bentonites has a number of potential safety-relevant impacts ranging from controls on the rates of mineral transformations, anion diffusivities, colloid filtration, radionuclide sorption, and Donnan effects on the swelling pressure (SKB 2011; Sections 8.3.2, 8.3.4, and 8.4.3.

Multiple-porosity models are based on the assumption that the following types of porosity can exist in compacted bentonites (Figure 2.4.2_1):

- interlamellar or interlayer porosity, which occupies the interlayer spaces of clay particles between individual tetrahedral-octahedral-tetrahedral (TOT) sheets (interlayer water is considered to be a few monolayers thick and may have different properties from bulk water due to its more structured nature); and

- external, or inter-particle, porosity, which includes spaces occupied by water in electrical double layers on the surfaces of clay particles as well as “free” water existing as interconnected thin films on the outside of clay stacks and on other bentonite minerals.

The amounts of each porosity type are believed to vary with compaction density. The external porosity decreases as compaction density increases. Diffusion of cations is envisaged to take place both through the interlamellar porosity and the external porosity, whereas anion diffusion takes place solely though the external porosity.

Single-porosity type models are based on the assumption that the buffer/backfill system consists essentially of only a single type of interlayer porosity, and that fluid compositions are controlled mainly by the Donnan equilibrium with an external solution and cation exchange (Birgersson and Karnland, 2009). Both cation and anion diffusion are assumed to be controlled by the interlayer pore diffusivity.

The effects of Donnan processes and anion exclusion are considered to be negligible in the SR-Site model of buffer/backfill geochemical evolution (SKB 2011, Sections 10.3.10 and 10.4.8; Sena et al., 2010) and in this sense the model seems to represent a multiple-porosity type model in which external porosity is homogeneously distributed and equal to the total porosity. Justification for this assumption comes from the good agreement claimed by Sena et al. (2010) between observed results for the transport of Cl^- and SO_4^{2-} in the LOT-A2 test parcel with corresponding modelling results obtained using a reactive-transport simulator (TOUGHREACT) that does not account for Donnan equilibria or anion exclusion. Although this justification may be valid, it would seem prudent from a reviewer's perspective to further explore the evident uncertainty and continuing debate concerning the nature of porosity in compacted bentonite. In particular, the Main Review Phase should evaluate, possibly on the basis of discussions with SKB, the potential impacts of alternative models of buffer/backfill geochemical evolution in which the possible existence of significant interlayer porosity and associated Donnan and anion exclusion effects are taken into account.

Any review during the Main Review Phase should, if necessary, include a component involving the use of alternative conceptual models and more comprehensive numerical models that can be used to independently evaluate the effects of bentonite microstructure on Donnan equilibria, anion exclusion and the geochemical evolution of the buffer/backfill. An example of such alternative numerical models is CrunchFlow (or CrunchFlowMC), which can be used to simulate mineral-water reactions and solute transport in the electrical double layer adjacent to clay-mineral surfaces (Steefel, 2009; Steefel and Maher, 2009)

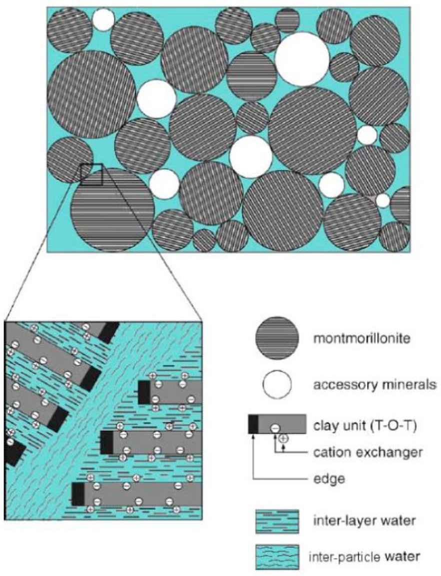

Figure 2.4.2_1. Schematic representation of the microstructure of compacted bentonite (from Sena et al., 2010, after Wersin, 2003)

2.5. Safety significance

The following questions were considered with regard to the safety significance of geochemical processes within buffer/backfill materials considered in SR-Site:

- Is the overall safety relevance of geochemical processes affecting the buffer and backfill explained and justified; and

- Is the safety assessment strategy for the handling of issues related to these processes clearly explained?

The present review assignment indicated that the safety relevance of geochemical processes within the buffer/backfill is in general adequately explained and justified, and that strategies for handling the effects of such processes are clearly explained in SR-Site and supporting documentation. Two concerns regarding this conclusion are discussed in the following subsections, however.

2.5.1. Retardation safety functions

The safety significance of certain modes of buffer/backfill failure is central to the selection of scenarios in SR-Site (SKB, 2011; Section 11). The focus of buffer failure scenarios is, however, primarily aimed at considering their impacts on subsequent canister failure. While prolonged containment is a feature of the KBS-3 concept, compliance with the SSM regulations concerns peak-risk/peak-dose of released radionuclides. Taking into account any future responses from SKB to the clarification requested in Section 2.1.3, SSM should therefore be prepared to consider in detail what might be the impacts of various buffer/backfill failure modes, and losses of safety functions, on the ‘retardation’ phase that follows canister failure (Appendix 3).

2.5.2. “CM” effects on safety function indicators

Geochemical processes affecting the buffer and backfill are treated in SR-Site generally in terms of potential changes in bentonite mineralogy (notably the montmorillonite content) and porewater chemistry (SKB, 2011; Sections 10.3.10; 10.4.8). On the other hand, the safety functions of these barriers are defined in terms of safety function indicators involving various physical and rheological properties, such as the density, swelling pressure and hydraulic conductivity.

The relation between (geo)chemical processes/properties (“C”) and (physical)/mechanical processes/properties (“M”) is not always clear. For example, although SKB have empirically established relations between montmorillonite content and swelling pressure for various bentonites (Karnland, 2010), it is less clear how changes in mineralogy, including re-distributions in mineral mass due to coupled reactive-transport processes, might locally affect the density, swelling pressure, and hydraulic conductivity, as well as other potentially important physical properties such as the stress/strain at failure. Although such relations are presently being evaluated in the LOT A2 investigations (Karnland et al., 2009; Olsson and Karnland, 2011), these experimental results can only provide qualitative insights concerning the extent to which CM effects might impact safety function indicators over time intervals that are relevant to the SR-Site safety assessment. Theoretical approaches to understanding the relation between geochemistry and mechanical/

rheological behaviour also do not appear to be well established at present. SSM should therefore be prepared to evaluate in further detail the relation between geochemical and mechanical processes that are likely to occur within buffer/backfill materials, and the effects of such CM coupling on corresponding safety function indicators (Appendix 3).

2.6. Transparency and traceability of information in SR-Site and associated references

This topic addresses whether information contained at different levels in the safety assessment (e.g., main SR-Site report, main supporting references, and other references) is internally consistent and logically subdivided. The present review indicated that with one exception (discussed below) all relevant information appears to be sufficiently consistent and adequately subdivided to justify further review of buffer/backfill geochemical processes during the Main Review Phase. The cross-referencing of information contained in the SR-Site report and main supporting references is adequate.

2.6.1. Access to information on computer codes, input/output files and supporting databases

SR-Site is based in part on numerical models of various geochemical processes that could occur within the buffer/backfill. The models are in general adequately described in SKB technical reports and scientific publications. This documentation may not be sufficiently detailed, however, that SSM could, if considered necessary, reproduce model results and evaluate the effects of alternative assumptions and parameter values. Although reference is often made to standard geochemical modelling software in such documentation, for example, the references rarely include information concerning specific 'release' versions of the software used (e.g., Sena et al., 2010). Similarly, input/output files used to evaluate the models are not generally provided. All assumptions underpinning the models may therefore not be completely transparent. References are generally given for thermodynamic, sorption and other fundamental databases supporting the models, but because these databases have been periodically revised it may not be clear and fully traceable regarding which databases were used, unless specific release numbers and release dates are provided.

Should SSM proceed to the Main Review Phase, it is recommended in the interest of full traceability and transparency that SSM should identify and request information to be provided by SKB concerning computer codes, input/output files and supporting databases used to support SR-Site. The information should be sufficiently detailed that SSM could, if necessary, reproduce model results, benchmark alternative numerical models, and evaluate sensitivities with respect to alternative conceptual models and parameter values (Appendix 3).

2.7. Feasibility of manufacturing, construction, testing, implementation, and operation

The descriptions of manufacturing, handling, and emplacement operations for the buffer and backfill are adequately summarized in SR-Site (SKB, 2011; Sections 5.5 and 5.6, respectively) and in the buffer and backfill production reports (SKB, 2010a and SKB, 2010b, respectively). Considerable work on developing these procedures has been carried out at the Äspö underground laboratory, and it is recognized that further refinement of such methods will necessarily require application and optimization at the Forsmark site itself.

The review raised a number of specific questions for which answers were not immediately apparent based on SKB's reporting. These questions are summarized in the following paragraphs.

Piping erosion is apparently to be treated by a "quantitative estimate with an empirical model" (SKB, 2011; Table 7.4.3). Details concerning this empirical model, especially with respect to how it will be qualified, and what counter-measures or changes in design, if any, SKB might consider if piping were found to be significant, are unclear.

Spalling is acknowledged to be a possible impediment to buffer emplacement (SKB, 2011; page 182) and seems to be attributable to immediate stress relief of the deposition hole surface. The likelihood of spalling, and possible remedial actions that could be taken if spalling were to occur during the actual buffer-ring emplacement (possibly arising from additional thermally induced stress to the rock surface (SKB, 2011; page 800) are unclear.

SKB expresses a concern for 'fast water uptake' of pellet-fillings (SKB, 2011; page 183), but it is unclear whether this concern is credible given the expected low hydraulic conductivity of the Forsmark host rock and possible long delay times in buffer re-saturation, possibly for most deposition holes.

Potential impacts from a maximum 13 MPa swelling pressure (SKB, 2011; page 187), such as on over-rigidity of the buffer in response to minor or major rock shear, are unclear.

3. Recommendations to SSM

The primary objective of this initial review assignment was to determine whether the documentation in SR-Site and supporting references is reasonably complete and of sufficiently high quality to justify a more detailed review of geochemical processes potentially affecting the safety functions of the buffer and backfill, and in particular to identify any complementary information and clarifications needed from SKB before such a review could be carried out. The SR-Site documentation relevant to this review topic was found to be of sufficiently high quality overall to justify further consideration in the Main Review Phase of SSM's PCS project. Several specific topics for which complementary information and clarifications should be requested from SKB were also identified (Appendix 2). Specific review topics for consideration during the Main Review Phase are recommended in Appendix 3.

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SKB 2010c. FEP report for the safety assessment SR-Site. SKB TR-10-45, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

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APPENDIX 1

Coverage of SKB reports

Table A:1 includes a list of SKB reports considered in the present review assignment. The list includes reports considered to be mandatory for review by SSM as well as additional relevant reports. Reviewed sections of the reports are indicated.

Table A:1 SKB reports considered in the review

Reviewed report	Reviewed sections	Comments
SKB TR-11-01: Long-term safety for the final repository for spent nuclear fuel at Forsmark	Sections 5.5, 5.6, 10.2.5, 10.3.7, 10.3.10 and 10.3.12	Reviewed revised versions of the main report obtained from SKB's website. Filenames: TR-11-01_VOLI_webb_ 2011-12.pdf; TR-11-01_VOLII_webb_ 2011-12.pdf; and TR-11-01_VOLIII_webb_ 2011-12.pdf (mandatory report)
SKB TR-10-47: Buffer, backfill and closure process report for the safety assessment SR-Site	Sections 3.5 and 4.4	(mandatory report)
SKB TR-10-45: FEP report for the safety assessment SR-Site	Appendix 6 and Appendix 7	(mandatory report)
SKB TR-10-15: Design, production and initial state of the buffer	Chapter 6	Reviewed a revised version of the report obtained from SKB's website. Filename: TR-10-15webb_2011-12.pdf (mandatory report)
SKB TR-10-16: Design, production and initial state of the backfill and plug in deposition tunnels	Chapter 6	(mandatory report)
SKB R-06-106: Assessment of the oxygen consumption in the backfill. Geochemical modelling in a saturated backfill	All	(relevant report)
SKB TR-10-60: Chemical and mineralogical characterization of the bentonite buffer for the	All	(relevant report)

control procedure in a KBS-3 repository		
SKB R-06-107: Effects of grouting, shotcreting and concrete leachates on backfill geochemistry	All	(relevant report)
SKB R-09-53: Characterisation of bentonite from Kutch, India and Milos, Greece – some candidate tunnel backfill materials?	All	(relevant report)
SKB TR-10-59: Aspects of geochemical evolution of the SKB near field in the frame of SR-Site	All	(relevant report)

APPENDIX 2

Suggested needs for complementary information from SKB

1. SKB should be requested to provide additional clarification concerning (Section 2.1.1):
    a. whether differences in processing techniques or refinements among various different bentonite suppliers to produce their 'as-delivered' material could directly or indirectly result in any adverse impacts on safety functions;
    b. whether differences in the exchange-site compositions of Ibeco RWC and MX-80 bentonites could significantly impact safety-relevant properties of the two bentonites (e.g., susceptibility to chemical erosion); and
    c. expected, as well as plausible, ranges in the Fe(III)/Fe(II) contents of montmorillonites in MX-80 and Ibeco RWC bentonites.
2. SKB should be requested to clarify why partial buffer transformation attributable to extraneous materials was not considered as a 'less probable' scenario to be calculated and included in the overall risk summation (Section 2.1.2).
3. SKB should be requested to provide clarification as to whether geochemical processes that could potentially affect retardation properties of the buffer and backfill in certain canister failure scenarios should be considered as 'less probable' scenarios to be calculated and included in the overall risk summation (Section 2.1.3).
4. SKB should be requested to provide clarification concerning the consistency of assumptions used in various geochemical models supporting SR-Site, including a description of all such models, identification of assumptions used in the models, a systematic analysis of inconsistencies among these assumptions, and identification of conditions for which any such inconsistencies can be considered unimportant (Section 2.1.4).
5. SKB should be requested to clarify their position concerning the importance of Donnan effects and anion diffusivities in models of both the swelling pressure and the geochemical evolution of buffer and backfill materials (Section 2.2.3).
6. SKB should be requested to address the following specific questions related to the feasibility of manufacturing, construction, testing, implementation, and operation of the buffer and backfill (Section 2.7).
    a. How will the empirical model to quantitatively estimate the extent piping erosion be defined and qualified, and what counter-measures or changes in design, if any, are envisaged should piping be found to be significant?
    b. What is the likelihood of spalling, and what possible remedial actions could be taken if spalling were to occur during buffer-ring emplacement?

c. Is the concern of “fast water uptake” by pellet fillings credible given the expected low hydraulic conductivity of the Forsmark host rock and possible long delay times in buffer re-saturation?

APPENDIX 3

Suggested review topics for SSM

1. SSM should carry out an independent technical evaluation of the pH < 11 safety function indicator criterion adopted in SR-Site (Section 2.2.1). The evaluation should consider established alternative methods to those adopted by SKB for the interpretation of smectite stability as a function of temperature, mineral chemistry and aqueous solution chemistry.
2. SSM should conduct a detailed review of SKB's SR-Site model of buffer/backfill chemical evolution (Section 2.2.2). If necessary, the review should include the development of an independent modelling capability that can be used to evaluate alternative conceptual models, underlying assumptions and parameter values.
3. If necessary depending on the adequacy of any clarifications from SKB concerning the importance of Donnan effects and anion diffusivities in models of the swelling pressure and geochemical evolution of buffer and backfill materials (Appendix 2), SSM should be prepared to conduct an independent, comprehensive and self-consistent evaluation of this issue (Section 2.2.3).
4. SSM should consider whether significant transformation of the mineralogy and physical properties of buffer/backfill materials due to indirect impacts from interactions with extraneous materials is possible, and, if so, whether such impacts should be considered as a less probable scenario that should be evaluated and included in the SR-Site overall risk summation (Section 2.4.1).
5. SSM should evaluate alternative conceptual models of buffer/backfill geochemical evolution that take into account the effects of bentonite microstructure on various types of porosity, and associated constraints imposed by Donnan equilibria and anion diffusivities (Section 2.4.2). The evaluation should, if necessary, include an independent modelling capability in order to evaluate the alternative models quantitatively using state-of-the-art reactive-transport simulation software.
6. SSM should evaluate the effects of various buffer/backfill failure modes, and losses of safety functions, on the 'retardation' phase following canister failure (Section 2.5.1).
7. SSM should evaluate the relation between geochemical and mechanical processes, and the effects of such CM coupling on safety function indicators for the buffer and backfill (Section 2.5.2).
8. Should SSM advance to the Main Review Phase, SSM should identify and request information to be provided by SKB concerning computer codes, input/output files and supporting databases used to support SR-Site. The information should be sufficiently detailed that SSM could, if necessary, reproduce model results, benchmark alternative numerical models, and evaluate sensitivities with respect to alternative conceptual models and parameter values (Section 2.6.1).

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The Swedish Radiation Safety Authority works proactively and preventively to protect people and the environment from the harmful effects of radiation, now and in the future. The Authority issues regulations and supervises compliance, while also supporting research, providing training and information, and issuing advice. Often, activities involving radiation require licences issued by the Authority. The Swedish Radiation Safety Authority maintains emergency preparedness around the clock with the aim of limiting the aftermath of radiation accidents and the unintentional spreading of radioactive substances. The Authority participates in international co-operation in order to promote radiation safety and finances projects aiming to raise the level of radiation safety in certain Eastern European countries.

The Authority reports to the Ministry of the Environment and has around 270 employees with competencies in the fields of engineering, natural and behavioural sciences, law, economics and communications. We have received quality, environmental and working environment certification.

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