COUPLED PROCESSES WORKSHOP REPORT

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ABSTRACT

To better prepare for a variety of possible future directions for the nation's nuclear waste program, staff are reviewing available literature on a range of geological media and conceptual repository designs. Geologic media, broadly categorized into crystalline, argillaceous, and salt rocks, are being considered as host media for radioactive waste disposal. Thermal-hydrological-mechanical-chemical (THMC) coupled processes can affect the ability of the host media and buffer/backfill materials to isolate the waste and mitigate the migration of radionuclides. Understanding these couplings of processes is essential for reliably assessing repository performance and evaluating the safety case. This report focuses on coupled THMC processes for geologic media (argillaceous, crystalline, and salt rocks) associated with emplacement of waste in deep underground facilities. Buffer, or emplaced engineered backfill, is added as a category because it is commonly a component of conceptual disposal designs, and analyses of coupled processes use similar tools to understand THMC conditions in the buffer and the rock. Much of the information in this report was presented and discussed in a U.S. Nuclear Regulatory Commission (NRC)/Center for Nuclear Waste Regulatory Analyses THMC workshop held March 31, 2011. Based on information available, staff identified the strongly coupled processes for each geologic media and buffer/backfill material. Determining which processes require strong linkage in a numerical code depends both on the ability to accurately model conditions observed in experiments and analogs, and the importance of the waste disposal design to performance. This information was used in the evaluation of capabilities and suitability of selected numerical models that could be used to simulate THMC processes in geologic media and buffer/backfill materials. Staff compiled information related to prominent laboratory and field tests that have a thermal perturbation component for argillite, buffer, crystalline, and salt as host rock. A survey of international projects supported NRC joining the Development of Coupled Models and Their Validation Against Experiments (DECOVALEX) group, whose goal is to increase understanding of THMC processes and validate models by simulating large laboratory or field experiments. Tasks for DECOVALEX-2015 starting in 2012 are currently under discussion by interested potential participants. Some of the tasks currently being proposed for DECOVALEX-2015 and related NRC considerations are discussed in this report.

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: None

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1 INTRODUCTION

The future direction of national policy for disposition of high-level radioactive waste is presently uncertain after the U.S. Department of Energy (DOE) petition to withdraw its license application for the construction of a repository at Yucca Mountain. The President of the United States chartered the Blue Ribbon Commission (BRC) on America's Nuclear Future to review options for managing the back end of the nuclear fuel cycle, including alternatives for storage, processing, and disposal. To become better prepared for a variety of possible future directions of the nation's waste program that may result from BRC panel recommendations, staff are reviewing available literature on a range of geological media and conceptual repository designs.

This report focuses on coupled thermal-hydrological-mechanical-chemical (THMC) processes associated with emplacement of waste in deep underground facilities. This THMC report is part of a series of closely related reports and workshops that are part of the Integrated Spent Nuclear Fuel Regulatory Activities (ISFR). Mined geologic disposal, rather than the deep borehole design, is considered in this report. Issues related to the deep borehole design are summarized in Winterle, et al. (2011a) and are not discussed here. The information in this THMC report overlaps with a recent report and a future workshop. First, this report overlaps with the salt report (Winterle, et al., 2011b) in that THMC processes related to salt are discussed here (Sections 2 and 4) to provide an expanded discussion of numerical modeling issues and approaches. A wider overview of issues related to a potential repository in salt host rock was presented in Winterle, et al. (2011b). Second, this THMC report and a planned future workshop on buffer materials overlap in that the former focuses on the near-field THMC environment in the host rock and buffer and the latter focuses more on the environment immediately surrounding a waste package and how that environment affects degradation of the waste package and waste form.

The purpose of this report is to summarize available information on coupled processes associated with deep disposal of waste in different geologic media. This report supplements and updates NUREG/CR–6021 (Manteufel, et al., 1993) on the fundamental equations for coupling THMC processes. The following three areas of information were not covered in the early NUREG document because of limited objectives of the report or because the information was not yet available.

- The present report identifies favorable attributes, and coupled processes important to barrier performance for three categories of geologic media and the engineered buffer. Manteufel, et al. (1993) focused on THMC processes in tuffaceous rocks.

- Whereas fundamental governing equations have not changed, constitutive relations for linking processes have advanced (e.g., change in porosity and permeability as the geomechanical stress field changes). In addition, computational capabilities have improved significantly over the past two decades, allowing larger and more complex problems to be simulated.

- Field and laboratory THMC experiments have been completed in granitic, argillaceous, and salt rock including experiments using bentonite buffers. International projects have used these experiments to improve and validate THMC numerical models.

The sections in the present report parallel these three areas. Section 2 identifies THMC coupled processes organized around each of three different categories of geologic media (granitic, argillaceous, and salt rock) and engineered buffer material. Section 3 discusses numerical modeling approaches for simulating coupled processes and lists codes used by different U.S. and international research groups. Section 4 summarizes field and laboratory experiments, especially those used to support understanding and modeling of THMC processes.

Much of the information in this report was presented and discussed in a U.S. Nuclear Regulatory Commission (NRC)/Center for Nuclear Waste Regulatory Analyses (CNWRA®) THMC workshop held March 31, 2011. The goal of the workshop was to provide background information to support NRC involvement in an international program on coupled processes in deep underground facilities. Another workshop goal was to disseminate information to NRC and CNWRA staffs to promote integration with other ISFR activities. A survey of international projects supported the choice of joining the Development of Coupled Models and Their Validation Against Experiments (DECOVALEX) group. The goal of the DECOVALEX project is to increase understanding of THMC processes and validate models by simulating large laboratory or field experiments. Participants choose to join one or more tasks depending on their priorities. The NRC/CNWRA workshop and this report were intended to help NRC decide which task(s) it might be interested in joining and decide whether there were additional components that NRC might propose for any task.

1.1 Background

The primary sources of information on THMC coupled processes are literature from international waste disposal programs, U.S. programs from the 1980s and earlier, and recent national laboratory activities (i.e., Sandia National Laboratories, Lawrence Berkeley National Laboratory, and Los Alamos National Laboratory). Corollary information is also available from studies in geothermal fields. An important source of information directly focusing on THMC processes for deep disposal of waste was a NUREG document created at the time NRC was joining the first phase of DECOVALEX in the early 1990s (Manteufel, et al., 1993). More recent documents of national and international program activities for deep disposal issues that cover THMC include IAEA (2003); OECD/NEA (2003); Hansen, et al. (2010a,b); Hansen and Leigh, (2011); Zhou and Arthur, (2010); and Liu, et al. (2010).

Early U.S. studies and international waste disposal programs in Europe and Asia cover a range of potential geologic media that can be categorized into crystalline, argillaceous, and salt host rocks because of similarities in coupled processes in each of these categories. Buffer, or emplaced engineered backfill, is added as a category because it is commonly a component of conceptual disposal designs, and analyses of coupled processes use similar tools to understand THMC conditions in the buffer and the rock.

The volume of buffer and host rock affected by excavation and emplacement activity is referred to as the near field. The near-field extent varies spatially and temporally depending on the THMC/HMC processes, properties of the host rock and buffer, and repository design. The host rock can be hypothetically divided into the far field and near field based on the extent of the THMC/HMC perturbation of the natural system. Although some of the general literature distinguishes between the excavation disturbed zone (EdZ) and the excavation damage zone (EDZ) (e.g., Tsang, et al., 2005), the distinction is not used in this report. In general terms, the EdZ includes the rock volume *without* significant changes to flow and transport properties, whereas the EDZ includes the rock volume *with* significant changes in flow and transport properties compared to the undisturbed host rock. Tsang, et al. (2005) describe different detailed definitions for each of four host rock types. In this report, the damage induced by the thermal perturbation is treated separately from damage induced by excavation.

1.2 Coupled Processes

This report includes a high-level overview of coupled processes in different geologic media. Because a fully coupled THMC model may be too computationally intensive, models that are more tractable may be created by identifying which processes should be intimately linked and which processes should be weakly linked. The latter may allow a simpler formulation to be implemented in the code, or the effect may simply involve adjustment of parameter inputs. Strong linkages may go both ways or just be unidirectional (e.g., thermal affects mechanical, but mechanical does not significantly affect thermal conditions). The judgment of which processes require strong linkage in a numerical code depends both on the necessity to accurately model conditions observed in experiments and analogs and on the importance to performance of the waste disposal design.

Identification of important coupled processes to strongly link in a numerical model depends on which geologic media are being considered. For example, (HM) processes may need to be coupled for argillites, but not for salt host rock. In addition, the importance of coupling in one direction may be more important than the coupling in reverse. For example, mechanical effects on hydrology may be more important than hydrologic effects on geomechanical performance.

Considering the four prominent processes of hydrology, geomechanics, thermal effects, and chemistry, there are 12 different couplings to potentially incorporate in analyses and modeling:

1.	Thermal	→	Hydrological
2.	Hydrological	→	Thermal
3.	Mechanical	→	Hydrological
4.	Hydrological	→	Mechanical
5.	Thermal	→	Mechanical
6.	Mechanical	→	Thermal
7.	Chemical	→	Thermal
8.	Thermal	→	Chemical
9.	Chemical	→	Hydrological
10.	Hydrological	→	Chemical
11.	Chemical	→	Mechanical
12.	Mechanical	→	Chemical

A visual summary of these 12 linkages for any geologic media is a quad-linear diagram as shown in Figure 1-1. This figure is a simple and succinct method to display the relative importance of different sets of coupled processes. Examples of how one process affects another process are added next to several of the arrows in Figure 1-1 to illustrate the concept of the figure. The figure does not represent any particular geologic medium, but is introduced here to avoid redundant explanations in Sections 2 and 3. In Section 2 of this report, a similar figure is synthesized for each of the four geologic media. The level of detail in the figures is sufficient for understanding decisions for implementing coupled processes in numerical codes. Thus, this type of figure is carried forth to the numerical code discussion in Section 3 of this report.

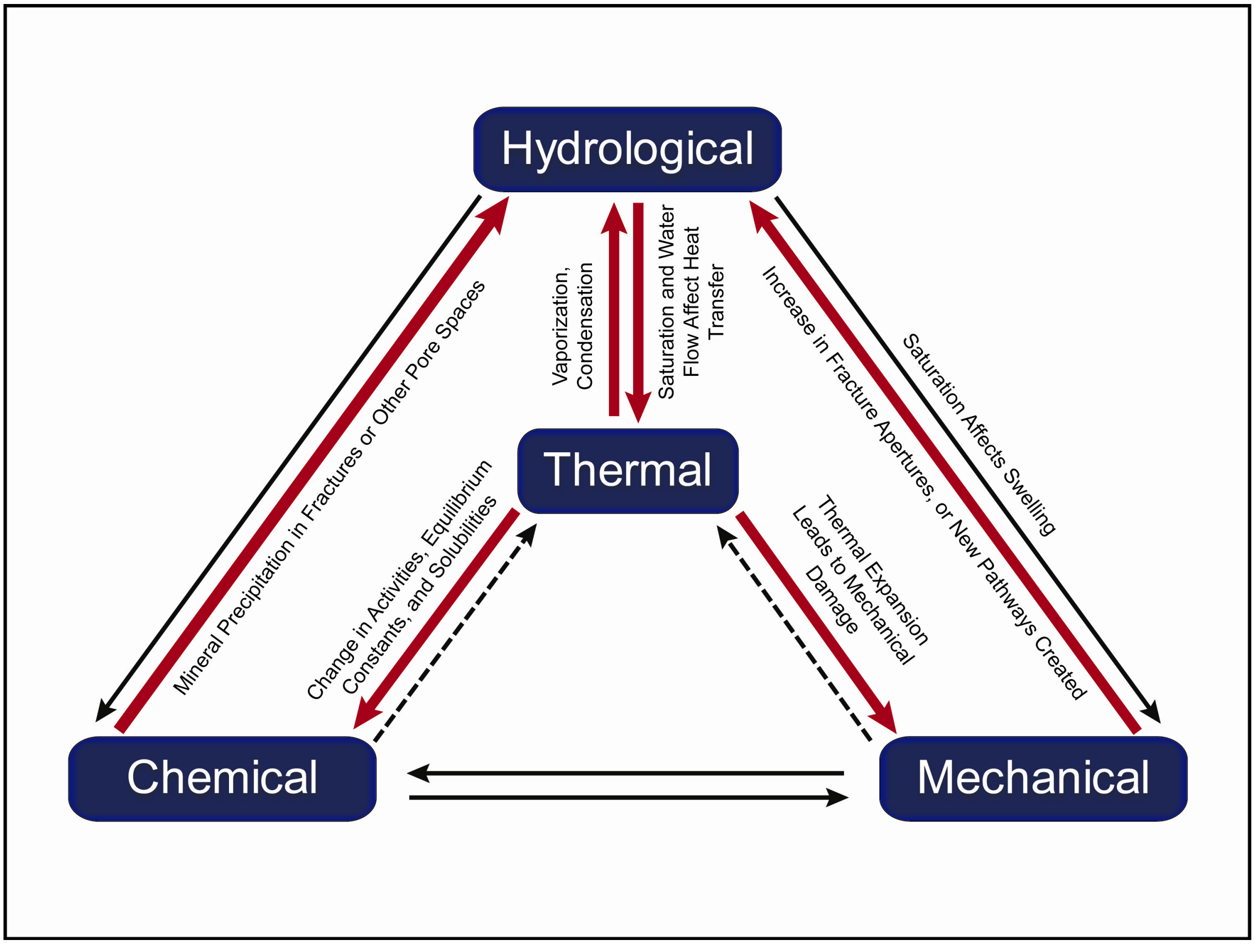

Figure 1-1. Example Diagram Illustrating Relevant Importance of Each Link for Coupled Thermal-Hydrological-Mechanical-Chemical Processes. Thick Red Solid Lines Indicate Strongly Coupled Processes, Thin Black Solid Lines Indicate Moderately Coupled Processes, and Dashed Black Lines Indicate Uncertain or Weakly Coupled Processes. Example Processes Illustrating the Coupling Are Provided Next to Some Arrows.

Radiation and biological processes are not included as separate processes for potential coupling with THMC in the near-field environment in this report (i.e., they are not considered for separate legs in the THMC framework of Figure 1-1). Radiation could lead to mineral alteration and radiolysis, which in the buffer or host rock could affect mechanical and hydrological conditions. For the first radiation-related process, direct mineral alteration, studies for buffer material or salt have been shown to have a negligible effect at the expected radiation levels (e.g., Posiva, 2007; Rothfuchs, 1985). The second radiation-related process, radiolysis, is the dissociation of water or other components by the ionizing radiation and consequent generation of gas and changes in water chemistry that may be more corrosive to engineered components. One approach for addressing radiation processes is to create design criteria limiting radiation at the outer surface of waste packages to keep radiation in the near field to an insignificant level, thus allowing radiation processes to be neglected in assessments (e.g., SKB, 2011; Posiva, 2007). In another approach, if a radiation-limiting design criteria is not incorporated into a repository design, the effects of radiation on the near field can be addressed in analyses of gas pressure increases (for gas generation) and in reactive transport models (for changes to water chemistry, including redox conditions). Radiolysis in the waste form environment in the waste package, however, may be important (IAEA, 2003; The National Academies Press, 2011), but is not in the scope of this report. For biological processes, the concern is microbial growth that may generate gas, alter water chemistry, and be a primary factor in controlling redox conditions (Wersin, et al., 2011). Microbial growth may increase the corrosive nature of water solution in contact with engineered barrier system (EBS) components, but likely would reduce the oxidative conditions (make more reducing) and thus reduce the solubility of radionuclides. As with radiolysis, gas generation from microbial activity can be indirectly factored into assessments by analyzing the effects of gas pressure buildup on hydrological and geomechanical conditions. For redox control by microbial activity, reactive transport models can be used with appropriate thermodynamic data (Tournassat, et al., 2011). In summary, gas pressure effects and chemical reactions from radiolysis and microbial activity can be incorporated in the THMC coupled models and can be factored into the discussions in Section 2 without adding separate legs for coupling models for radiation and biology.

Prior to excavation of a repository, groundwaters at repository depths would be in a reducing environment. During repository construction, the introduction of air would result in an oxidizing environment. As resaturation proceeds, this oxygen will be consumed by processes including container corrosion, reaction with minerals, and microbial processes. The evolution of the reducing-oxidizing environment (redox) likely will depend to a large extent on waste container corrosion processes and on the supply of redox sensitive species from the surrounding host rock. Redox mainly is dependent on chemical reactions (typically involving ferrous iron, sulfides, or organic carbon). Temperature affects reaction rates and hydrology affects flow of oxygenated waters, implying that coupled THC processes indirectly affect redox conditions. Hence, evolution of redox conditions is not discussed further in this report.

1.2.1 Design

At the level of detail needed for this report, only high-level information on design is necessary. As mentioned earlier, deep borehole disposal is not considered here. THMC processes associated with emplacement directly in drifts or in large boreholes vertically or horizontally spaced along drifts or tunnels are considered. Figures 1-2 and 1-3 are examples from the Swedish and French waste disposal designs. Figure 1-2 shows both the vertical (KBS-3V) and horizontal (KBS-3H) designs. Both have a bentonite buffer and a backfill of the access drift. The primary difference for THMC processes is that the backfill for the vertical emplacement design may play a larger role in affecting temperature and hydrologic conditions.

One other design consideration that may prominently affect THMC processes is the thermal management strategy. To maintain flexibility, thermal criteria used by several European countries are acknowledged but not used to constrain the discussion in Section 2. Complex THMC processes could potentially lead to degradation of EBS and host rock, supporting a design temperature limit to be maintained below boiling {e.g., 90 °C [194 °F]} at all times. The effects of temperatures above boiling are considered in the discussion in Section 2.

1.2.2 Performance

An understanding of the evolution of the near-field environment is needed to explain the importance of THMC processes for repository performance. Figure 1-4 provides an example of the evolution for argillaceous host rock and includes a qualitative time frame for the processes. For designs with bentonite buffer, salt rock, and argillaceous rock, containment of waste over

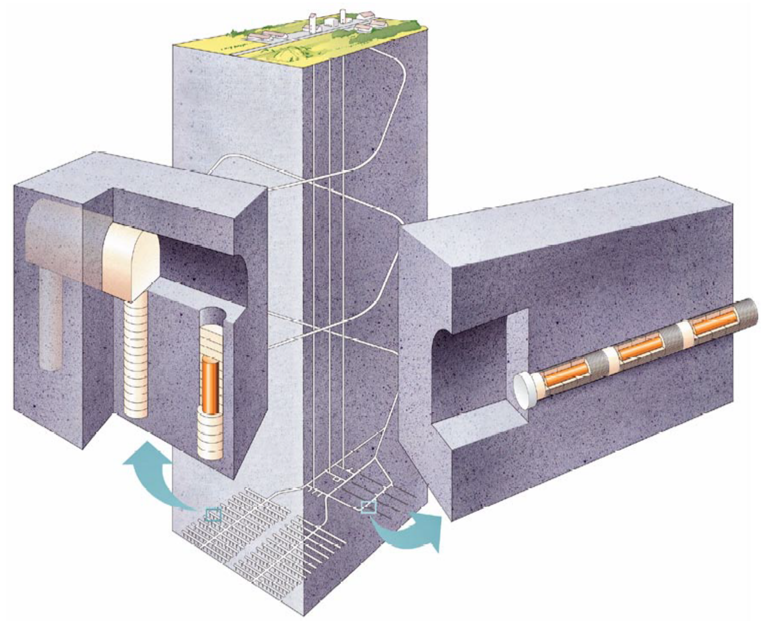

Figure 1-2. Example of Vertical (KBS-3V) and Horizontal (KBS-3H) Emplacement Design from Access Drifts from the Swedish Waste Disposal Program (SKB, 2010, Figure 16-1). (Reproduced With Permission From SKB. Illustration by Jan Rojmar.)

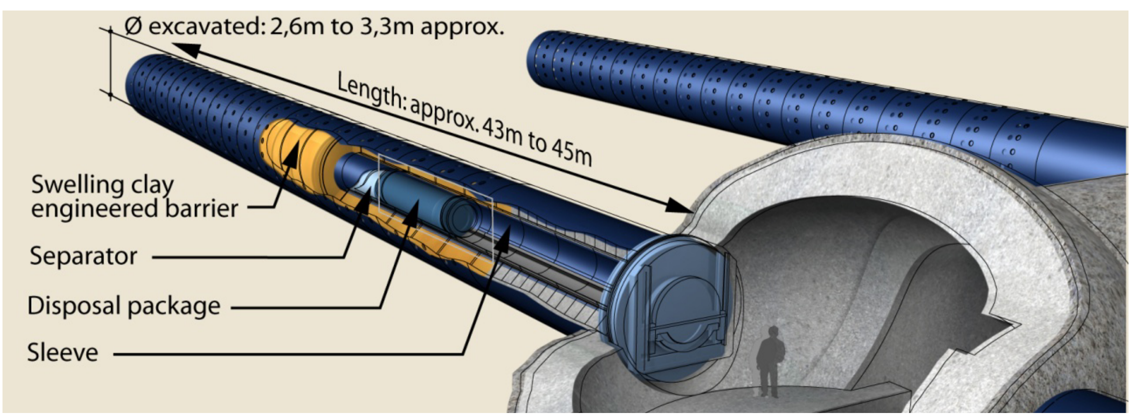

Figure 1-3. Example of Horizontal Emplacement Design from Access Drifts for Spent Fuel from the French Waste Disposal Program (ANDRA, 2008). (Reproduced With Permission From ANDRA). [1m = 3.28 ft])

long periods relies on stabilization of hydrological, mechanical, and chemical conditions. In effect, the geologic media theoretically reseal, or close transport pathways in the near field and radionuclides do not reach the far field except by diffusion. The timeframe for diffusional transport of radionuclides is long, in tens to hundreds of thousands of years, for distance scales in the tens of meters [1 m = 3.28 ft]. For deep underground disposal, distances through the far field to the biosphere are much greater than the tens of meters [1 m = 3.28 ft]. A containment period of hundreds of years achieves some benefits in terms of activity reduction for short-lived radionuclides. If containment degrades after hundreds of thousands of years, the radionuclide activity is significantly reduced by decay of short-lived radionuclides (e.g., Cs-37 and Sr-90) and some smaller benefit is achieved by a more limited amount of decay of long-lived radionuclides. Dispersion and sorption further reduce the activity reaching the biosphere.

However, during the thermally perturbed period when only short-lived radionuclides have exhibited significant decay, hydrological, mechanical, and chemical conditions are also perturbed. Depending on the excavation damage, emplacement design (e.g., thermal management strategy), and the thermal properties of the geologic media, the thermal period may last from hundreds to tens of thousands years. In this perturbed environment, advective water may contact the waste package, and chemical conditions conducive to corrosion of waste packages could lead to waste dissolution and advective radionuclide transport through the near field.

The importance of THMC processes to repository performance must be determined for the synthesis of figures similar to Figure 1-1. Manteufel, et al. (1993) created a hierarchy of importance for THMC processes for the proposed Yucca Mountain repository. The BENCHPAR project (Stephansson and Min, 2004) illustrated the use of judgment of a THM collaborative group to identify levels of importance using benchmark tests to support the rankings of different inputs and conditions. Other studies on performance for THMC processes are also qualitatively based on modeling efforts for different geologic media (e.g., Sellin and Alheid, 2008). Note, however, that performance and safety cases in other countries may rely on subsystem metrics, instead of the risk-informed, total performance approach found in the current U.S. regulation for a proposed repository at Yucca Mountain. In light of these comments, Figures 2-1, 2-3, 2-4, and 2-5 are syntheses of staff's judgment based on information from available literature.

1.3 Organization of Report

Section 2 contains subsections for each of the four media: argillaceous, granitic, and salt host rock and buffer. The subsections summarize attributes of each geological medium important to waste isolation and describe important coupled processes that should be considered in analyses and numerical codes used to predict system behavior and performance. Section 3 describes numerical modeling approaches and existing codes for different sets of processes while considering the needs of the different geologic media. High-level options are suggested for developing in-house THM and THC capabilities for numerical codes. Information on these two approaches—existing codes and development of in-house capabilities—is presented with the intention of laying out options for future decisions on the direction of the program. Future direction could include either approach or a combination of the two. Section 4 contains a summary of thermal tests associated with underground facilities with appropriate references. Section 5 presents a report summary.

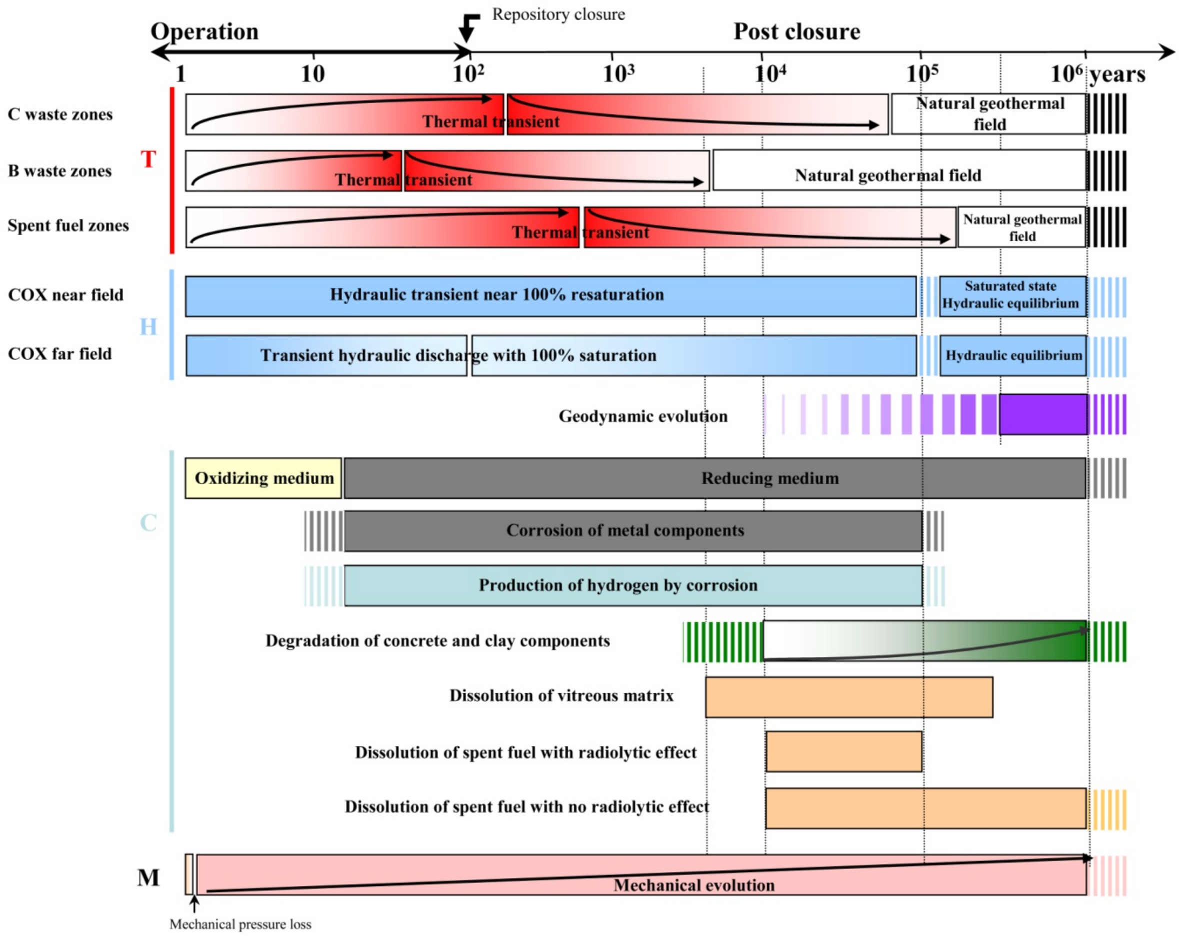

Figure 1-4. Time Scales for Thermal-Hydrological-Mechanical-Chemical Processes for Deep Disposal in Argillaceous Host Formation (ANDRA, 2005, Figure 4.3.1). (Reproduced With Permission From ANDRA). C-Waste—High-Level Waste, B-Waste—Intermediate/Low-Level Waste, and COX—Callovo-Oxfordian Clay.

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2 COUPLED PROCESSES IN DIFFERENT GEOLOGIC MEDIA

An overview of coupled processes in different geologic media is presented in this chapter. The focus is on the evolution of (i) thermal-hydrological-mechanical-chemical (THMC) coupled processes associated with the heat load imposed on the geologic media by the emplaced radioactive waste and (ii) HMC coupled processes during the postthermal period until the repository reaches steady-state conditions. Experience in many other countries over the last 20 to 30 years has shown that acceptable disposal conditions can be found in such diverse rock types as granitic rocks, metamorphic rocks, plastic clays, indurated clay stones, salt domes, and sedimentary formations. These types have been commonly categorized into argillaceous rocks, crystalline rocks, and salt (IAEA, 2003). The host media are expected to contribute to the safety of disposal by playing three main roles: (i) isolating wastes from the near-surface environment and the potentially disruptive processes that occur there; (ii) maintaining a geochemical, hydrogeological, and geomechanical environment favorable to the preservation and performance of the engineered barrier system (EBS); and (iii) acting as a natural barrier restricting the access of water to the wastes and the migration of mobilized radionuclides (IAEA, 2003). The relative importance of the three roles varies in different host media. Significant variations are possible and depend on the nature of the host rock and the design of the repository. Thus, for a repository in hard crystalline rock, roles (i) and (ii) are likely to be the most important, while for a repository in salt deposits or argillaceous sediments, role (iii) is expected to dominate.

The host media have different properties that are both favorable (e.g., high sorption and low dissolution in argillaceous formations) and unfavorable [e.g., very low sorption for salt (Table 2-1)] to repository performance. During the thermal period, the heat load may affect (i) flow conditions in the host rock that, in turn, influence water reaching the repository and transport in the repository; (ii) the stress distribution in the host rock that determines the mechanical integrity of structures, distribution of fractures, and hydrologic properties of fractures; (iii) geochemical conditions that may alter hydrologic properties; and (iv) microbial activity that, in turn, influences corrosion and radionuclide transport (IAEA, 2003). Understanding these couplings of processes is important for a reliable assessment of repository performance and for the evaluation of the safety case. The next sections discuss the coupled processes in argillites (Section 2.1), buffer/backfill and cementitious materials (Section 2.2), crystalline rocks (Section 2.3), and salt (Section 2.4).

Table 2-1. Properties of Potential Host Media Relevant for Disposal*

Property	Salt Formations	Crystalline Rocks	Argillaceous Formations
Thermal Conductivity	High	Medium	Low
Permeability	Practically impermeable	Very low (unfractured) to permeable (fractured)	Very low to low
Deformation Behavior†	Visco-plastic (Creep)	Brittle	Plastic to brittle
Strength	Medium	High	Low to medium
Dissolution Behavior†	High	Very low	Very low
Sorption Behavior†	Very low	Medium to high	Very high

*German Federal Ministry of Economics and Technology. "Final Disposal of High-Level Radioactive Waste in Germany—The Gorleben Repository Project." Berlin, Germany. 2008
†Does not include changes because of thermal perturbation.

Favorable | Average | Unfavorable

2.1 Coupled Processes in Argillites

Argillaceous clay-rich formations, such as plastic and indurated clays, shale, and mudstone, are considered as potential repository host rock because of their favorable hydrologic (low permeability), chemical (low diffusion coefficient, high retention capacity for radionuclides), and mechanical properties (capability to self-seal fractures in the damaged zone) (Table 2-1). These formations exhibit a wide range of types: from plastic clay deposits, with transitional types, to strongly consolidated and partially fractured clay deposits. The range of types can be associated with considerable differences in deformation behavior, temperature sensitivity, and rock strength. In the absence of open fractures and advective flow, diffusion is the dominant transport mechanism for radionuclides in argillaceous formations. The heat pulse causes complex mechanical, hydraulic, and chemical interactions in the host rock, and all phases (gas, liquid, solid) need to be considered (OECD/NEA, 2003).

The influence of the excavation damage zone (EDZ) in both indurated and plastic clays on barrier capability of the host rock has been evaluated in international programs (Tsang, et al., 2005). The EDZ has been identified as a potential preferential pathway for flow; however, flow in the EDZ is limited by the availability of water from the surrounding argillaceous formations.

Based on current staff understanding, the interaction of THMC processes for argillites is conceptualized in Figure 2-1. The dominant linkages for argillites include the (i) TH coupling that refers to the influence of thermal load on the rate of saturation and desaturation processes; (ii) TC coupling that refers to the temperature-dependent chemical characteristics such as solubility and sorption coefficients and clay mineral and colloid stability; (iii) TM coupling that influences the rate of swelling (thermal expansion); and (iv) HM coupling that refers to the influence of saturation on development of pore pressures that, in turn, control the swelling process.

2.1.1 Thermohydrological Processes

Temperature regimes above boiling in argillites may lead to complex hydraulic phenomena driven both by the high temperatures and high temperature gradients. The hydraulic processes may be affected by mechanical phenomena that are also driven by high temperature gradients and by increased chemical reactivity of argillites as temperatures rise above boiling (ANDRA, 2005a). Thermal convection effects in clay are generally not expected because of its relatively low permeability. However, the formation of convection cells is also dependent on the repository geometry and the induced temperature gradients in the clay formation (OECD/NEA, 2000, 2003).

The dominant heat transfer mechanism is conduction in the host rock. Owing to their planar layer, argillaceous formations (e.g., Callovo-Oxfordian layer) may exhibit strong anisotropy in their ability to transfer heat (thermal conductivity) in the horizontal versus the vertical direction (ANDRA, 2005a). The anisotropy (horizontal: vertical) ratio in thermal conductivity for Callovo-Oxfordian clay was estimated to be 1.5. The impact of this anisotropy is most prominent in the near field during the initial thermal period and diminishes as the thermal load dissipates.

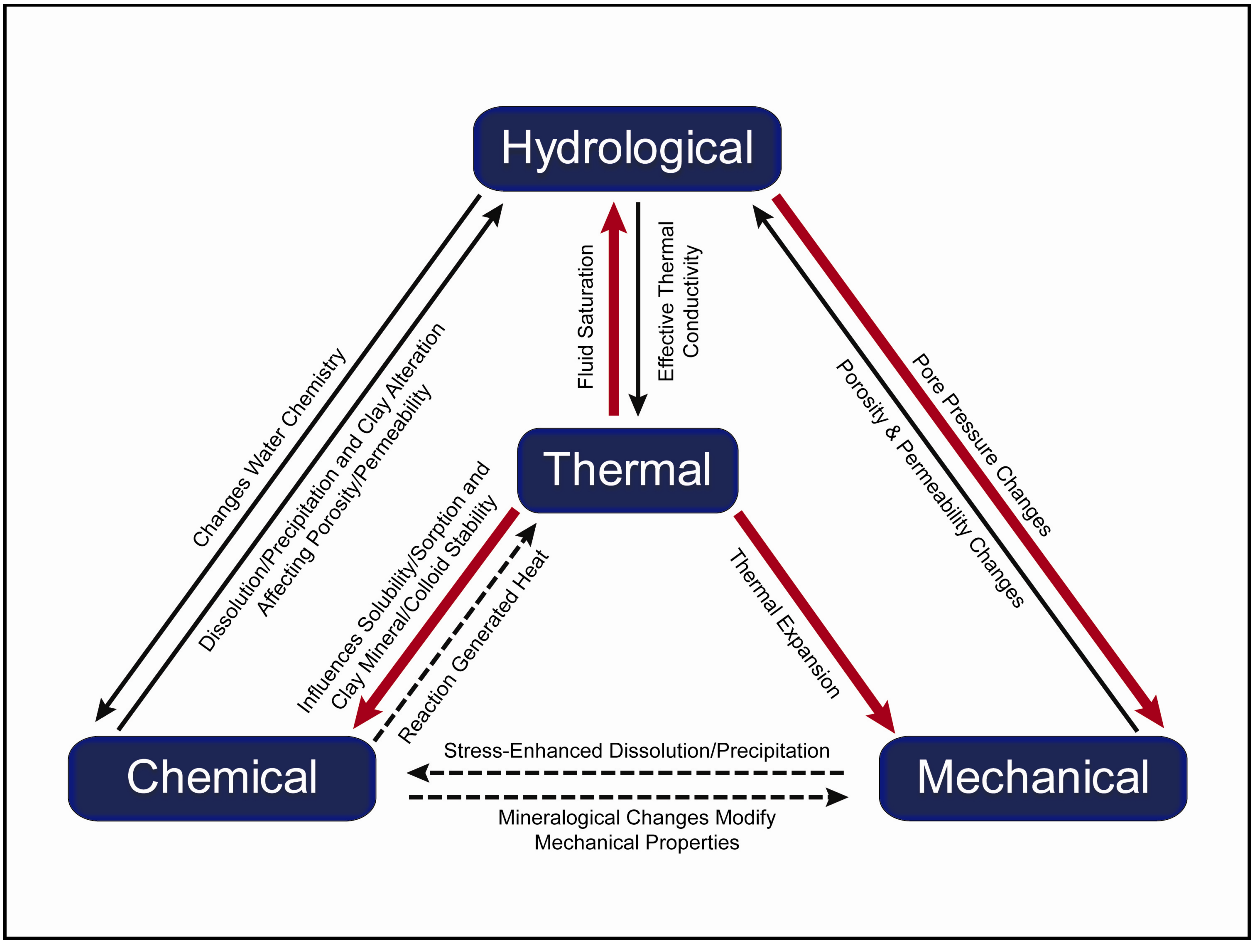

Figure 2-1. Conceptualization of Thermal-Hydrological-Mechanical-Chemical Interactions for Argillites

The processes that influence the hydrologic regime in the near field are as follows (ANDRA, 2005a):

- Hydraulic head drop and desaturation during the construction/operating phase
- Resaturation of the repository
- Return to saturated hydraulic equilibrium

The excavation and construction operations lead to a rapid drop in the hydraulic pressures of the geological formations in the immediate periphery of the tunnels or drifts, shafts, access ramps, or other structures (commonly known as the “hydraulic head drop”). The ventilation of the underground structures leads to a pressure gradient that results in a radial convergent flow into the structures. The duration and rate of flow depends on the hydrologic properties of the surrounding formations. The anisotropy in permeability also influences the rate of the hydraulic pressure drop. The relatively low permeability values of argillites imply that the desaturation rate caused by ventilation spreads at a much slower rate compared to hydraulic head drop. Once the postclosure operations are completed (i.e., closure and sealing of all underground structures) and the heat load from the emplaced waste decreases, the desaturation process ceases and transitions into a resaturation process. The gradual resaturation process of the near field will continue until a state of hydraulic equilibrium with the far field is reached.

The hydrologic properties of the host rock (mainly permeability and porosity) control the rate of desaturation and resaturation. Characterization of the host rock with low permeability (hydraulic conductivity to water of approximately 10^{-8} m/s [1m = 3.28 ft] and smaller) may require additional considerations, such as high precision instrumentation and ensuring that the hydraulic gradient imposed during testing is appropriate for measurement (ANDRA, 2005a; Neuzil, 1986). Too high a gradient could lead to modification of the porosity due to the hydraulic and mechanical coupling and turbulent water flows. Low permeability host rocks also imply that electro-osmosis, thermo-osmosis, and chemical osmosis could influence the flow. Production and migration of hydrogen released by corrosion and vapor (in case of above-boiling conditions) could also influence the hydrologic conditions.

2.1.2 Geochemical Processes

The significant temperature difference between *in-situ* argillite host rock and the emplaced waste may affect the favorable properties (e.g., low hydraulic conductivity, swelling capacity, and sorption) of the host rock. Possible effects include (i) transformation of smectite to illite that could lead to an embrittlement and a partial or total loss of swelling capacity; (ii) dissolution/precipitation reactions and clay mineral alteration that could change the hydraulic conductivity of the argillite; (iii) changes in the pore water chemistry that could affect radionuclide solubility and sorption, waste package corrosion, and waste form degradation; (iv) modification of the ion-exchange, hydration, and swelling behavior of the clay minerals; and (v) alteration of clay colloid stability. Degradation of organic material also could occur and lead to production of CO_2 or monocarboxylic acids, which, in turn, could (i) change the pore water pH and ionic strength; (ii) dissolve carbonate minerals; and (iii) change ion-exchange equilibria, clay surface properties, and radionuclide speciation and sorption. As illustrated in Figure 2-1, temperature could have a significant effect on clay mineral/colloid stability and radionuclide solubility and sorption, whereas chemical processes, such as dissolution/precipitation reactions and clay alteration, could modify the hydrologic properties of the argillite host rock. On the other hand, water chemistry in the near field could be changed by flow of groundwater with different composition.

Experimental data, natural analog information, and chemical model calculations indicate that heating to 85 or 95 °C [185 or 203 °F] for a few hundred years is insufficient to cause significant chemical or mineralogical changes in argillites like Opalinus Clay (Mazurek, 2002). The basin analysis by Leu, et al. (2001) showed that Opalinus Clay has experienced an 85 °C [185 °F] temperature for at least 20 million years, but smectite is still present in the rock, demonstrating the long-term stability of the clay mineral. Results of short-term (1 year) tests at 90 °C [194 °F] using Boom Clay and Opalinus Clay specimens showed that limited mineral alteration resulted from the thermal–chemical perturbations of the tests, at least within the timeframe of the study by Honty, et al. (2010). The most significant change observed in that study is the oxidation of pyrite accompanied by sulfate release and dissolution/precipitation of carbonate and gypsum. Also, no significant variations were observed in the measured cation-exchange capacity of the Boom Clay and Opalinus Clay in the course of the experiments. However, Honty, et al. (2010) cautioned against extrapolating the short-term test results to repository conditions, which will span longer time periods than the duration of the experiment. In addition, temperatures significantly higher than 90 °C [194 °F] could increase the rate of chemical or mineralogical changes of argillite.

2.1.3 Geomechanical Processes

Geomechanical processes result from activities or occurrences that change the state of stress in the repository host rock. Activities, such as excavation of repository openings, and occurrences, such as heat release due to radioactive decay, change the rock stress. Rock excavation consists of removing the static support the excavated rock previously provided. As a result , the stress state in the surrounding rock changes, and the rock deforms to adjust to a new equilibrium state. Thermal load from the disposed waste causes the rock to try to expand by different amounts at neighboring points because of spatially varying temperature. However, the potential expansion is partially suppressed by different amounts in different directions due to neighborhood resistance, resulting in nonuniform increase in rock stress. The rock deforms as a result to adjust to a new equilibrium state. Additionally, the thermal load causes any pore fluids to try to expand by different amounts at neighboring points because of spatially varying temperature, which results in pore pressure increase if the fluids cannot flow freely. The excess pore pressure changes the rock stress and loading conditions, and the rock deforms to adjust to a new equilibrium state. The excess pore pressure dissipates with time at a rate that depends on the fluid conductivities, compressibility of the solids skeleton, and distance to drainage boundaries. Additionally, drainage at the excavated opening causes changes in pore water pressure and could cause rock near the opening to desaturate. The resulting pore pressure or suction changes cause a change in the rock stress and loading conditions, and the rock deforms to adjust to a new equilibrium state.

Each activity or occurrence, such as those described in the foregoing paragraph, causes the rock to deform. The deformation could be elastic and, therefore, fully reversible, or inelastic. Inelastic deformations may be expressed through formation of new cracks, slip or opening or closing of existing cracks, or particle morphology changes not associated with cracking. If inelastic deformation is dominated by cracking, as may occur in stiff overconsolidated clays (e.g., Gens, et al., 2007), the cracks could coalesce to form spatially persistent or connected fractures that may constitute paths for faster fluid flow. In contrast, if inelastic deformation is dominated by particle morphology changes without cracking, then existing cracks could heal and result in partial closure and disconnection of previously connected fractures, thereby disrupting some existing through-going flow paths (e.g., van Geet, et al., 2008). Also, inelastic deformation could cause rock to converge toward the openings by amounts large enough to increase loading on ground support or cause external loading of waste containers. The potential for inelastic deformation and the deformation magnitude and type (e.g., brittle, ductile, expansive, or contractive) depend on mechanical characteristics of the host rock and the type of activity, such as excavation, or magnitude of an occurrence, such as thermal load.

2.1.3.1 Deformations Due to Excavation

Excavation of an opening could result in a damaged rock zone (referred to as EDZ) near the boundaries of the opening. The EDZ consists of zones of macro- or microfractures that extend into the rock from the opening to a distance that depends on several factors. The factors that affect the EDZ extent and damage intensity include the *in-situ* stress magnitude; rock mass strength and stiffness; orientation of the openings relative to the orientations of the *in-situ* stress and any structural discontinuities or mechanical anisotropy, such as bedding planes; and method of excavation. For example, van Marcke and Bastiaens (2010) describe observations and measurements at the Belgian underground research laboratory that indicate two sets of fractures formed due to excavation of horizontal tunnels in a soft plastic clay known as Boom Clay. The fractures suggest an EDZ that extends about 1.0 m [3.28 ft] radially and 6 m [19.7 ft] axially beyond the tunnel end for a 4.8-m [15.8 ft] diameter circular tunnel.

The EDZ extent and damage intensity also could be affected by water pressure changes due to the excavation, if the excavation is below the water table. For an excavation below the water table, pore pressure changes due to drainage or stress effects cause a change in rock stress and force distribution, which result in deformations that could affect the EDZ development. The effect of water pressure is potentially more important in argillaceous rocks because of the low hydraulic conductivity and, therefore, slow rate of dissipation of excess pore water pressure. Conversely, fracturing could enhance the hydraulic conductivity within the EDZ, therefore increasing the dissipation rate of excess pore water pressure. The increase in hydraulic conductivity could increase drainage enough to reduce the magnitude, extent, and duration of excess pore pressure, thereby reducing the EDZ growth. Conversely, an increase in effective stress could cause a decrease in hydraulic conductivity within the EDZ because of fracture healing, as was indicated by laboratory testing of Opalinus clay samples from the Mont Terri rock laboratory in Switzerland (Jobmann, et al., 2010).

2.1.3.2 Deformation Due to Saturation Changes

Because of their clay mineral content, argillaceous rocks could shrink if the degree of saturation decreases, or swell if saturation increases. Saturation may decrease near the excavation boundaries because of rapid drainage following excavation or moisture loss due to ventilation. A decrease in saturation at values of water content between the liquid limit and shrinkage limit of the argillaceous rock will cause shrinkage and, potentially, cracking or fissuring due to shrinkage (e.g., Peron, et al., 2009). The potential shrinkage strain appears proportional to the change in water content relative to the liquid limit (e.g., Peron, et al., 2009). Desaturation may cause cracking if the potential shrinkage cannot occur because of boundary constraints or nonuniform changes in water content (e.g., Peron, et al., 2009). Investigations of a candidate repository site in the Callovo-Oxfordian argillites (ANDRA, 2005a, Section 8.3.2.2) suggest that cracking or fissuring due to desaturation is not likely to extend more than a few tens of centimeters [1 cm = 0.4 in] into the rock from an excavation boundary. Also, laboratory testing of Opalinus clay specimens showed shrinkage and surface cracking due to drying (Soe, et al., 2009). Swelling during resaturation may reverse the effects of desaturation such as shrinkage and cracking. For example, tunnel wall observations reported in ANDRA (2005a, Section 8.3.2.2) indicate shrinkage fissures close as relative humidity in the tunnel increases. Also, saturation changes affect mechanical properties of argillaceous rocks because of desiccation and the effects of saturation on suction. The rock strength and stiffness increase due to desaturation but decrease as the rock absorbs water to return to a saturated state.

2.1.3.3 Deformation Due to Thermal Load

Thermally induced deformation could occur due to suppressed thermal expansion of solids and pore fluid. Potential thermal expansion is partially suppressed because of nonuniform heating of the rock mass (i.e., rock temperature change due to heating from disposed nuclear waste varies spatially and temporally). Suppressed thermal expansion of solids causes thermal stress that causes deformation as the rock adjusts to a new equilibrium state. The resulting thermal stress has deviatoric and pressure components that vary with the magnitude and gradient of temperature change and the mechanical boundary conditions. Also, suppressed thermal expansion of water causes an increase in water pressure in saturated rock (cf. Gens, et al., 2007). The excess water pressure changes the rock stress and water force distribution, and the rock deforms to adjust to a new equilibrium state. Deformation due to suppressed pore water expansion is likely to be important in saturated argillaceous rocks because of low permeability. For example, measurements in Opalinus clay at the Mont Terri underground research laboratory (Kull, et al., 2007) indicate that pore water pressure increased from a range of 0.7–1.2 MPa [102–174 lbf/in^2] to 3–4 MPa [435–580 lbf/in^2] within a distance 0.8–1.4 m [2.6–4.6 ft] from the test heater. As the data showed, the pore pressure increase varied spatially and temporally and could be greater at locations outside the immediate neighborhood of the heater. Thermally induced pore pressure in argillaceous rock could be large enough to cause microcracking because the water is contained in pores with low-permeability linkage. Therefore, thermally induced fracturing of a saturated argillaceous rock could result from the combined effects of stress increase due to suppressed thermal expansion of the solids skeleton and pore pressure increase due to suppressed expansion of pore water.

2.2 Coupled Processes in Buffer and Backfill

The EBS represents the man-made, engineered materials placed within a repository, including the waste form, waste canisters, buffer materials, backfill, and seals of access tunnels and drifts (OECD/NEA, 2003). Depending on the repository design, the EBS could play a significant role in the containment and long-term retardation of radionuclide release. Bentonite or a bentonite–sand mixture is proposed as a buffer and backfill material in a number of countries (IAEA, 2003; NWTRB, 2009). The hydrological (low hydraulic conductivity), geochemical (very low diffusion, high sorption, good colloid and microbial filtration capability), and mechanical (high swelling potential enables self-sealing of openings) properties of bentonite make it a favorable buffer/backfill material between the waste packages and host rock.

There are several EBS design options being considered in international waste disposal programs. They include vertical (Figure 2-2) and horizontal configurations (Figure 1-3) for the EBS. Though the terms buffer and backfill are sometimes used interchangeably, some EBS design options (as shown in Figure 2-2) use both buffer and backfill. The functions of the buffer can be broadly described as (i) providing physical, chemical, hydrologic and biological isolation; (ii) minimizing radionuclide release; and (iii) protecting the canisters from rock displacements (especially in the case of crystalline rocks) (OECD/NEA, 2003, Table 3-4). The functions of the backfill include (i) isolating the EBS hydrologically from other shafts and access routes; (ii) keeping the buffer in place; (iii) restricting buffer swelling/expansion upwards; and (iv) keeping the tunnels mechanically stable (OECD/NEA, 2003, Table 3-4; Posiva, 2006; SKB, 2011). The effectiveness of the buffer strongly depends on its swelling pressure as this feature influences its barrier capability. Swelling pressure is affected mainly by the density of bentonite and by the groundwater salinity. A loss of swelling pressure would lead to increased hydraulic conductivities in the near field and potentially decreased canister lifetime.

The evolution of the buffer and backfill can be characterized as follows (Steefel, et al., 2010; SKB, 2011; Posiva, 2006):

<u>**Construction and Operation Period**</u>

During the construction and installation phase, the buffer could be partially saturated. Wetting of the buffer could occur based on the local conditions. The wetting process is slow because of the low permeability of the bentonite and the surrounding host rock (either crystalline or argillaceous formations). Fracture-dominated flow in crystalline rocks could result in uneven wetting of the bentonite because it is dependent on the active fracture network at the bentonite–rock interface. For argillaceous rock, fracture flow is potentially less significant and wetting of the bentonite could be controlled by inflow from the rock matrix. The buffer and backfill material may not have developed sufficient swelling pressure at this stage. For

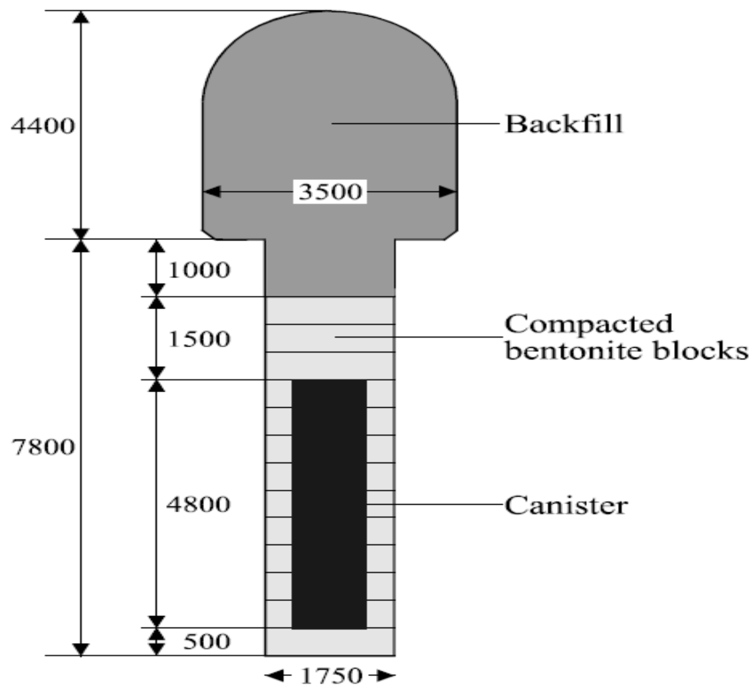

Figure 2-2. Example of a Vertical Engineered Barrier System Configuration Consisting of Both Buffer (Compacted Bentonite Blocks) and Backfill (Posiva, 2006). (Reproduced With Permission From Posiva Oy).

repository sites that could experience inflow of water to the open repository (e.g., SKB, 2011), the potential for piping and associated erosion effects on the buffer and backfill need to be evaluated. Piping may lead to erosion of bentonite. This erosion may lead to a lowered density in certain parts of the buffer and backfill and may affect the barrier capability of buffer and backfill. The swelling properties of bentonite make the buffer and backfill material swell and close open gaps or channels to form a more homogeneous buffer or backfill. Buffer components (e.g., bentonite blocks, pellets) and gaps need to be homogenized (heterogeneity to be limited) for buffer/backfill to serve as an effective isolation barrier.

Thermal Period

The second phase is dominated by heat input from the waste canister with a significant time-varying temperature gradient, with the temperature initially increasing and then returning to ambient conditions. The initial pore water in the buffer will be redistributed during early thermal phases. At the buffer–host rock interface, water is absorbed from the surrounding host rock, with potential bentonite swelling in this region. At the buffer–waste package interface, moisture content decreases (desiccation) with potential shrinkage. The temperature gradient and degree of saturation in the buffer affect the temperature and moisture distribution during the resaturation process. Chemically, dissolution and precipitation of secondary minerals may occur within the buffer.

Postthermal Period

During this phase, the thermal gradient will decrease as the temperatures approach the ambient conditions. The resaturation rate will be dominated by the hydraulic gradient in the buffer. The buffer and the backfill are expected to reach close to 100 percent saturation during this period. The backfill is expected to saturate before the buffer because of buffer's high degree of compaction and exposure to higher temperatures from the emplaced waste.

Long-term Performance

During this period, tectonic or glacial processes under ambient or reduced temperature conditions determine the buffer and backfill performance significantly. The effect of coupled processes on long term repository performance depends on the repository site and is not evaluated in detail in this report.

Based on current staff understanding, the interaction of THMC processes for the buffer is conceptualized in Figure 2-3. The dominant linkages include the (i) TH processes that affect the spatial and temporal distribution of the saturation during the drying and rewetting of the buffer during the initial postclosure period; (ii) the degree of swelling that is controlled by the HM coupling with a strong impact of the thermal pulse; (iii) the THC/TC coupling that determines the chemical composition of the buffer that impacts the retardation capabilities of the buffer (sorption, solubility, colloid properties); and (iv) the TCM coupling that could cause changes in mechanical properties for above-boiling conditions.

2.2.1 Thermohydrological Processes

Water initially contained in the buffer near the canister surface will evaporate and migrate away from it by vapor diffusion, followed by condensation in the outer part of the buffer or at the rock surface (OECD/NEA, 2003; Posiva, 2006; SKB, 2011). The buffer surface close to the canister thus remains essentially dry (unless artificially wetted at emplacement time) until the buffer is slowly saturated from the outside during or after the operational phase. The heat transfer rate is sensitive to local conditions (e.g., gaps around the bentonite, water content of bentonite). The rates of wetting and drying are very slow in the buffer because of its low hydraulic conductivity. For example, MX-80, a buffer material proposed to be used in several international programs (SKB, 2011), has a hydraulic conductivity of 10^{-12} m/s [1 m/s=3.3 ft/s].

Water saturation of bentonite and the development of a swelling pressure are important to dissipate the heat generated by the emplaced waste. Wetting increases the buffer thermal conductivity, and the swelling of the buffer eliminates the gaps. The dominant heat transfer mechanism in (i) solids (buffer) is conduction, (ii) liquid-filled gaps (between the buffer and host rock) is convection, and (iii) air-filled gaps (gap between the waste canister and buffer) is radiation. A solid contact between interfaces of solid materials (waste canister, buffer, rock) is most favorable because air gaps act as barriers to heat transfer. Therefore, achieving water saturation and maximum swelling pressure in the buffer and backfill as soon as possible will enable (i) faster heat dissipation and (ii) restoration of the low hydraulic permeability. A high swelling pressure is also needed as soon as possible to protect the canister from microbially induced corrosion (Posiva, 2006).

If the heat load is sufficiently high to cause above-boiling temperatures, steam generation during the buffer resaturation period can induce a significant volume reduction of the clay, which can occur even at relatively short times of contact with steam at 110 °C [230 °F] (OECD/NEA, 2000). Hydrothermal field tests showed considerable cementation of the clay, causing brittleness and loss of expansion within a few centimeters [1 cm = 0.4 in] of the steel

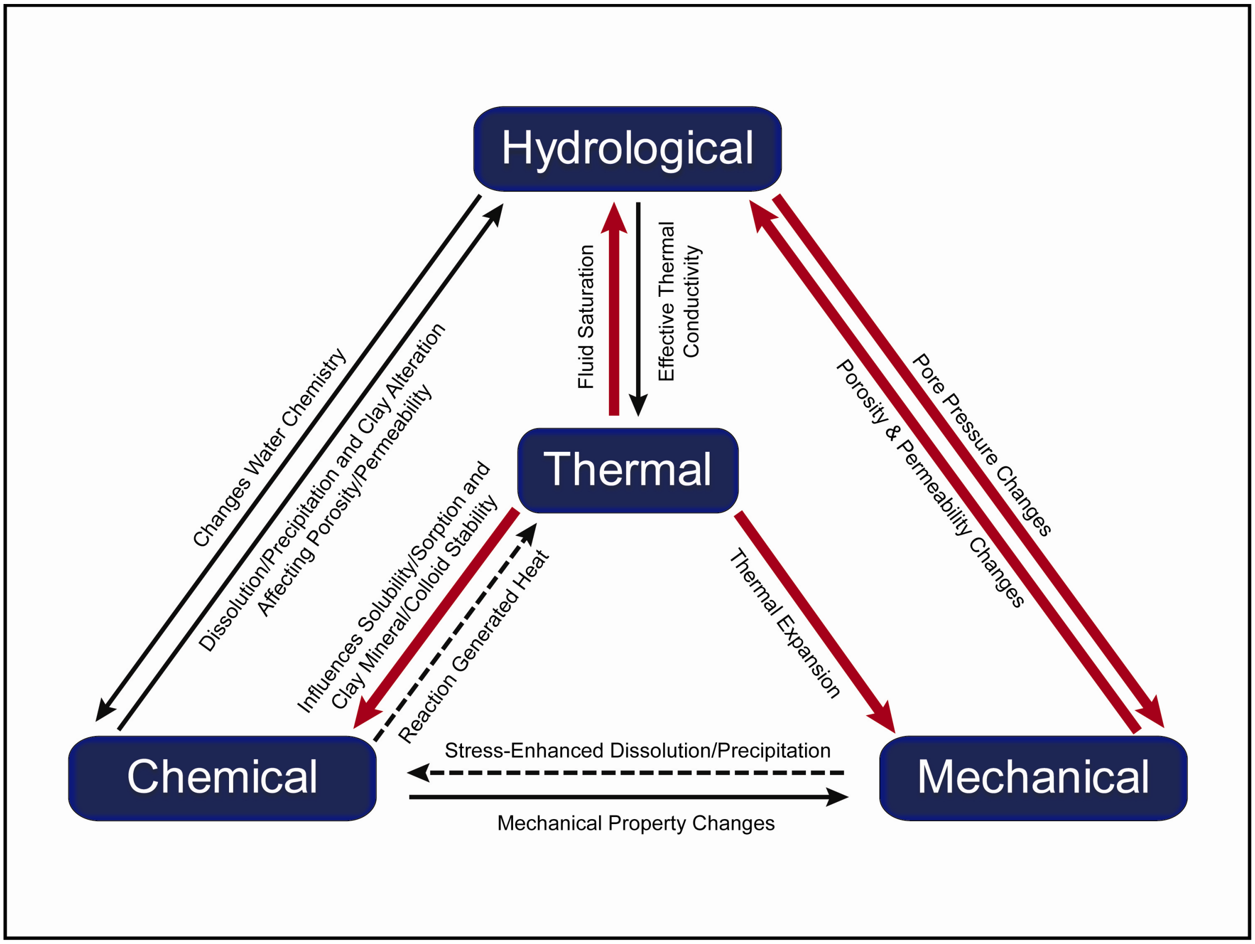

Figure 2-3. Conceptualization of Thermal-Hydrological-Mechanical-Chemical Interactions for Buffer

surface of the heat source (Pusch and Börgesson, 1992). In the hottest region, anhydrite and hexa-hydrate were precipitated, probably attributable to their retrograde solubility (i.e., these phases are less soluble at higher temperatures). Slightly farther away from this hottest zone, new amorphous silica–aluminum phases formed in this slightly cooler region. The mobilization and deposition of these phases may be attributable to their solubility in a thermal gradient or to cyclic evaporation and condensation that take place in resaturating clay under a thermal gradient. Gas was also found to have filled interior voids of the backfill, probably water vapor dominantly, although some hydrogen gas may have evolved from corrosion of the steel heater in the field test. Thus, complex THMC processes that could potentially lead to degradation of the EBS (i.e., bentonite buffer) support a design temperature limit to be maintained below boiling at all times.

2.2.2 Geochemical Processes

The equilibrium states of chemical reactions vary with temperature and reaction rates increase with temperature. Thus, chemical or mineralogical changes in the bentonite buffer/backfill could occur due to heating in the near field. The main thermal–chemical effect on bentonite may be heat-induced transformation of montmorillonite to either beidellite or illite, depending on the concentration of dissolved K^+ ion. Low K^+ concentration leads to the formation of beidellite, which exhibits similar expansion properties as montmorillonite and does not collapse permanently with cations other than K^+ in its interlamellar spaces (OECD/NEA, 2003). At high K^+ concentration, nonexpanding illite mineral forms. Transformation of montmorillonite to illite in the bentonite buffer/backfill could lead to embrittlement of the material, a partial or total loss of swelling capacity, and an increase in hydraulic conductivity of the clay material (Karnland and Birgersson, 2006).

Higher temperatures also could enhance dissolution/precipitation reactions (e.g., involving silica or calcite) that could alter the hydraulic conductivity and possibly create preferential flow paths in the bentonite buffer/backfill. For example, dissolution of silica has been observed to be significant at temperatures exceeding 150 °C [302 °F] and its precipitation has been observed to occur on cooling during hydrothermal testing of Na-montmorillonite (Andersson, 1989). Calcium in the groundwater may react with carbonate in the bentonite and precipitate calcite. Calcite precipitation is enhanced by higher temperature because its solubility decreases with increasing temperature. Silica or calcite precipitation may block pores in the bentonite buffer/backfill and reduce its elastic properties.

Higher temperatures due to waste emplacement also could cause (i) changes in the pore water chemistry that could affect radionuclide solubility and sorption, waste package corrosion, and waste form degradation; (ii) modification of the ion-exchange, hydration, and swelling behavior of the clay minerals; and (iii) alteration of clay colloid stability. In addition, degradation of organic material and production of CO_2 or monocarboxylic acids could be enhanced, which, in turn, could (i) change the pore water pH and ionic strength; (ii) dissolve carbonate minerals; and (iii) change ion-exchange equilibria, clay surface properties, and radionuclide speciation and sorption (OECD/NEA, 2003).

As illustrated in Figure 2-3, the chemical properties of the buffer/backfill material could be altered by mechanical and hydrologic processes. Mineral dissolution and precipitation could be enhanced by elevated stress imposed on the buffer/backfill material, and water chemistry in the near field could be altered by flow of groundwater with different composition.

2.2.3 Geomechanical Processes

Potential geomechanical processes in a buffer or backfill are similar to the geomechanical processes in argillaceous rock (Section 2.1.3), because buffer and backfill compositions include appreciable amounts of clay minerals that may swell or shrink due to a water content gain or loss. However, the geometry and boundary conditions of buffer or backfill designs differ from the geometry and boundary conditions for argillaceous host rock. As discussed in Section 2.1.3, buffer and backfill may undergo elastic and inelastic deformations; the inelastic deformation may be expressed through formation of new cracks, slip or opening or closing of existing cracks, or particle morphology changes not associated with cracking. Inelastic deformation in a buffer or backfill could result in (i) coalescence of small cracks to form spatially persistent fractures that may constitute paths for faster fluid flow or (ii) partial closure of existing cracks, thereby preventing such cracks from connecting with other cracks to form faster flow paths.

Buffer or backfill deformations may be driven by thermal loads or water influx from the host rock. Thermal effects on buffer and backfill deformation may consist of free or partially suppressed thermal expansion of the solids skeleton or pore water, shrinkage due to desiccation in areas experiencing thermally driven moisture loss, swelling in areas experiencing thermally driven moisture gain, or other deformations due to thermally induced changes in stress or suction.

Deformations due to water influx consist primarily of swelling, but may include collapse for loosely compacted material or the effects of material property changes, such as particle crushing due to wetting (e.g., Alonso, et al., 1990).

Buffer deformations need to be evaluated to assess potential changes that could affect the capability of the buffer to reduce advective transport. The evaluation needs to consider cracking due to desiccation, crack healing due to swelling, evolution of the desiccation front, cracking due to loss of vertical confinement, internal erosion of the buffer, and buffer failure at the canister base or foundation. Backfill deformation may need to be evaluated to assess potential external loading of contiguous engineered barrier mechanical components.

Cracking Due to Desiccation

A fine-grained soil could crack during desiccation if the potential drying shrinkage cannot occur and results in a tensile stress equal to the tensile strength of the material. As Peron, et al., (2009) discussed, partial suppression of drying shrinkage could arise from the effects of displacement boundary restraints, nonhomogenous moisture content, stress concentration due to geometrical features or material nonhomogeneity, or intrinsic factors, such as soil texture and structure. Buffer designs contemplated for geologic repositories (e.g., SKB, 2011; Rutqvist, et al., 2001; Hokmark, et al., 2007) include features such as structural gaps that may reduce desiccation cracking and features that may increase its occurrence. A key feature of buffer designs that could increase the potential for desiccation cracking is the moisture gradient that results from the buffer being exposed to a persistent heat source on one boundary and groundwater influx at the opposite boundary.

Simultaneous moisture loss from the heated area and gain near the exterior boundary creates a moisture gradient through the buffer that could persist for a long time. Such a condition could result in nonuniform shrinkage and tensile stress.

Crack Healing Due to Swelling

Fine-grained soils, especially soils that include clay minerals such as montmorillonite, swell as the moisture content increases. If the boundary is constrained or the moisture content is nonuniform, a part of the potential swelling is suppressed and pressure develops in the soil as a result. Soil swelling potential depends on mineralogy, dry density (e.g., Ye, et al., 2010), confining stress, and overconsolidation ratio (i.e., ratio of the vertical yield stress to the vertical *in situ* stress). Soil swelling could result in crack healing because a swelling soil deforms to occupy any available open space such as cracks. For example, laboratory testing (van Geet, et al., 2008) of fracture sealing in natural clayey soils due to an increase in confining stress suggests that the potential for sealing is high for soft clays and relatively low for stiff clays. Contemplated buffer designs for geologic repositories (e.g., SKB, 2011; Rutqvist et al., 2001; Hokmark et al., 2007) include features that could enhance free swelling (e.g., structural gaps and using bentonite as a primary constituent), features that could suppress swelling (e.g., persistent moisture gradient), and at times a specification of a minimum swelling pressure (e.g., SKB, 2011). The effectiveness of such designs for sealing potential cracks needs to be evaluated.

Evolution of the Desiccation Front

Buffer design concepts anticipate placement of the buffer material in an initially unsaturated state (e.g., SKB, 2011). The saturation subsequently will decrease in buffer areas close to the canister because of evaporation and moisture migration away from the heat. Also, saturation is expected to increase in areas of the buffer close to the host rock because of water influx from the host rock and moisture migration from hotter to cooler areas and condensation in the cooler areas. Dixon, et al. (2002) describe measured moisture content distributions in a buffer dismantled after a heating experiment that show relatively dry conditions near the heater and wetter conditions as distance from the heater increases. Based on the understanding described in this paragraph, the buffer is expected to become dryer in areas close to the canister and wetter in areas close to the host rock, which implies a desiccation front or boundary occurs between dryer and wetter buffer areas. This front could migrate through the buffer with time depending on the heat output rate from the canister, groundwater flux from the host rock, and buffer dimensions and properties. The configuration of the desiccation front could be used to estimate the buffer zones subjected to conditions that may permit desiccation cracking.

Cracking Due to Loss of Vertical Confinement

If the buffer contacts the host rock in a configuration that permits development of vertical shear stress, the vertical compressive stress at a point in the buffer could conceivably decrease below values consistent with the weight of overlying materials because vertical stress is transferred to the host rock through friction. Such load transfer could result in horizontal fracturing of the buffer. A vertical contact between the buffer and host rock creates a favorable condition for the occurrence, but the small height of the buffer may reduce the potential for the occurrence. This mechanism was believed to have contributed to leakage problems in several rockfill dams with clay cores during the period of 1960–1980 (e.g., Sherard, 1973).

Internal Erosion of Buffer

Internal erosion of the buffer could occur if water flows through a channel (e.g., connected cracks) with a velocity high enough to erode the channel walls. SKB (2011, Section 6.2.2) identifies “mechanical erosion” as a potential failure mechanism for a buffer. The erosion channel could initiate due to high flow velocity through connected fractures or loosely compacted material. If the eroded material could be dispersed into host rock fractures, then the channel through the buffer could grow into a permanent feature. Alternatively, the eroded material could be deposited at the buffer–rock interface and slowly clog the channel. Internal erosion was identified as a potential failure mechanism for earth dams that could be reduced by providing a filter zone on the downstream side of the clay core (e.g., Sherard, 1973).

Buffer Failure at Canister Foundation

In combination with thermal stress, pore water pressure, and swelling pressure, stress due to canister weight could cause excessive deformation of the underlying buffer, such that the canister could sink into the buffer. SKB (2011, Section 6.1.2) identifies canister sinking due to consolidation or creep of the buffer as a potential interaction between a canister and buffer. The diffusion barrier under the canister base could deteriorate or reduce in thickness if parts of the buffer under the canister deform excessively. However, the potential occurrence of this buffer failure mechanism can be assessed using either a procedure for geotechnical evaluation of punching failure of foundations or a procedure based on coupled analysis of stress, deformation, and pore pressure.

2.2.4 Coupled Processes in Cementitious Material

Cementitious materials are major components of engineered barriers or structures in most low-level waste (LLW), intermediate-level waste (ILW), and transuranic (TRU) waste geologic disposal repositories and in some high-level waste (HLW) repository concepts [e.g., Belgian *Supercontainer* concept (Bennett and Gens, 2008)]. These materials are used in repository vaults, floors, tunnel linings and plugs, waste conditioning matrices, and backfill. In LLW and ILW repositories, cementitious materials are relied upon to serve as chemical and physical barriers to radionuclide release and transport. This reliance is based on the ability of cementitious materials to buffer the pH of infiltrating water to ≥12.5, which lowers the solubility of certain radioelements and decreases the corrosion rate of carbon steel that may be used for waste containers. Where blast furnace slag is used as a supplementary cement material, the slag induces a reducing geochemical environment in which redox-sensitive radioelements, such as technetium, exhibit low solubility and high sorption. In addition, cementitious materials have low permeability that reduces groundwater flow and radionuclide transport, and the cement minerals provide sorption sites that could retard radionuclide migration. For HLW repositories, the functions and requirements of cementitious materials listed in Table 2-2 indicate that cementitious materials are relied upon as barriers to groundwater flow due to their low permeability and for structural support of repository openings due to their mechanical strength.

Because of the alkaline pH of cement pore waters, interaction with crystalline and argillite host rocks and with clay buffer/backfill is an important geochemical process that needs to be considered in performance assessments. The alkaline pH of cement pore waters could alter the host rock mineralogy and buffer/backfill properties. Dissolution and precipitation processes could occur and result in porosity/permeability changes that alter groundwater/gas flow pathways in the host rock and buffer/backfill. For example, dissolved carbonate ions in solution are known to react with calcium in the cement to form calcite and seal the pores or fractures in the cementitious material or in the adjacent rock.

Interaction of groundwater with cementitious materials also could change the water chemistry and affect radionuclide solubility and sorption. Vitrified waste form dissolution is expected to be faster at higher pH, although spent fuel dissolution rates likely will be unaffected by alkaline solutions. Also, interaction of alkaline solutions with clay minerals would produce a variety of reaction products, such as brucite and zeolites.

Knowledge Gaps and Future Work

There are significant uncertainties in the intensity and extent of interaction between cement leachates and surrounding barriers; in particular, bentonite-type backfill and buffer materials. There is also uncertainty in the intensity and extent of perturbation of the host rock by the alkaline plume and in the resulting changes in chemical and hydraulic containment capacities of the repository system. Although “low-pH” cements (i.e., cement formulations that result in pore water pH ≈ 11) have been developed to help mitigate the effect of alkaline plume interactions with near-field components, limited data are available on the long-term performance and durability of low-pH cements in contact with groundwaters. Pilot-scale tests on low-pH cement emplacement have been conducted, but further testing is needed under environmental conditions similar to repository conditions. There is a need to demonstrate that the low-pH cements will not have a negative effect on bentonite in the long term.

Table 2-2. Functions and Requirements of Cementitious Material Components in a High-Level Waste Repository*			
Components	**Functions**	**Preclosure Requirements**	**Postclosure Requirements**
Structural liner	Ensure mechanical stability of tunnels and shafts	Mechanical strength	No detrimental effects on other barriers
Grout backfill	Provide contact between liner and host rock; suppress water inflow	Low permeability	No detrimental effects on other barriers
Fracture grouting	Suppress water inflow through fractures	Low permeability	No detrimental effects on other barriers
Mechanical plug	Confine and mechanically support backfill material	Mechanical strength	No detrimental effects on other barriers
*Metcalfe, R. and C. Walker. "Proceedings of the International Workshop on Bentonite—Cement Interaction in Repository Environments." NUMO–TR–04–05. Tokyo, Japan: Nuclear Waste Management Organization of Japan. 2004.			

Chemical models have greatly improved over the last 10 years to enable simulating chemical processes occurring both within the concrete and between the concrete and other surrounding materials such as bentonite. However, further work is needed to enable upscaling models of cementitious materials to larger temporal and spatial scales; in particular, porosity–permeability changes because of precipitation/dissolution processes. Another major challenge is how to couple chemical evolution with changes in mechanical properties of cementitious repository materials.

Additional work is also needed to better understand radionuclide aqueous speciation, the potential importance of colloids, and the effect of cement additives such as superplasticizers, which are chemical additives that increase the fluidity of the cement or concrete mix without producing excess water. Plasticizer degradation may form reaction products that may complex and mobilize radionuclides but few data are available on this process. In addition, plasticizer formulations are evolving and likely would change during the period of repository planning. Further experimental studies are needed to understand the potential effect of plasticizers on radionuclide mobilization and transport. Also, information is needed on the radionuclide solubility controlling phases in cementitious materials and on radionuclide sorption behavior under chemical conditions affected by cementitious materials.

Heat will affect the chemical evolution and mechanical properties of cementitious materials. The effects of temperature on cement chemistry are known in general terms, but these are not fully described or quantified. Temperature may also have a strong influence on mechanical behavior, especially with regard to processes such as creep, shrinkage, and cracking. It is difficult to describe and model these processes at any particular temperature and more so under thermal gradients.

2.3 Coupled Processes in Crystalline Rocks

Crystalline rocks, such as granite and gneiss, are considered for their hydrogeological (low permeability in unfractured rocks), mechanical (high strength), and geochemical characteristics (high sorption and low dissolution) that are beneficial to repository performance.

Depending on the degree of connectivity of the fractures in the rock, the dominant radionuclide transport mechanism is advection with some potential diffusive transport. The flow regime in crystalline rocks is governed by the extent of fracture connectivity and presence of structural features such as faults. The influence of the EDZ in crystalline rocks on barrier capability of the host rock has been evaluated in international programs (Tsang, et al., 2005). The potential for connected fast flow paths in the EDZ, the impact of EDZ on resaturation rate (especially of the buffer), and the role of EDZ at tunnel intersections are some of the issues that could impact long-term barrier capability.

Based on current staff understanding, the interaction of THMC processes for crystalline rock formation is conceptualized in Figure 2-4. The dominant linkages include (i) TMH coupling which influences the thermal deformations that, in turn, could lead to changes in permeability and porosity; (ii) TH coupling that influences the thermal conduction processes; and (iii) TC coupling that influences the solubility and sorption properties of the host rock.

2.3.1 Thermohydrological Processes

The dominant heat transfer mechanism is conduction. The thermal perturbation leads to the creation of thermo-convective cells in fractures and faults (ANDRA, 2005b). The potential of formation of thermo-convective cells is restricted by fracture network geometry, particularly continuity and connectivity. Continuity of structural features refers to extent (length) of a single feature, whereas connectivity refers to fractures or faults intersecting other fractures or faults. Shorter fractures or faults are less likely to be interconnected with other structural features. Flow in a fault network depends on the fault dimension, orientation, and connectivity with other faults. Most repository design approaches, however, avoid major faults within the repository footprint. The temperature of the far field is largely controlled by the natural geothermal gradient, although it may be influenced by heat output from the repository and by changing climate at the surface. The heat generated in the repository will be dissipated by conduction through the rock mass and, to a much lesser extent, by advection in the moving groundwater.

Consequently, the thermal impact of the repository will reduce with distance from the near field (IAEA, 2003; ANDRA, 2005b). The anisotropy in the thermal properties, if significant, should be evaluated because it determines the spatial and temporal distribution of temperature in the host rock.

The processes that influence the hydrologic regime in the near field for crystalline rocks are similar to the argillaceous formation (ANDRA, 2005b; SKB, 2011; Posiva, 2006): (i) hydraulic head drop and desaturation during the construction/operating phase; (ii) resaturation of the repository; and (iii) return to saturated hydraulic equilibrium. The excavation and operation of the repository could result in hydraulic and hydrogeochemical disturbances, such as the drawdown of the water table, surface water intrusion and upconing of saline water and increase in salinity. Upconing, or the localized inducement of vertical flow, may lead to marked changes in salinity or other chemical changes in the water in the vicinity of the emplacement zone. The potential for a large influx of groundwater into the repository during the construction and operating phase can be addressed to some extent by grouting and type of excavation equipment (Posiva, 2006; Tsang, et al., 2005). During the early postclosure period, the rapid initial inflow is followed by an asymptotic regime where the inflow gradually decreases. It is expected to take several hundred years for the repository to reach full saturation because of the low hydraulic conductivity of crystalline rocks (~10^{-13} – 10^{-14} m/s [1m = 3.28 ft]) (SKB, 2011).

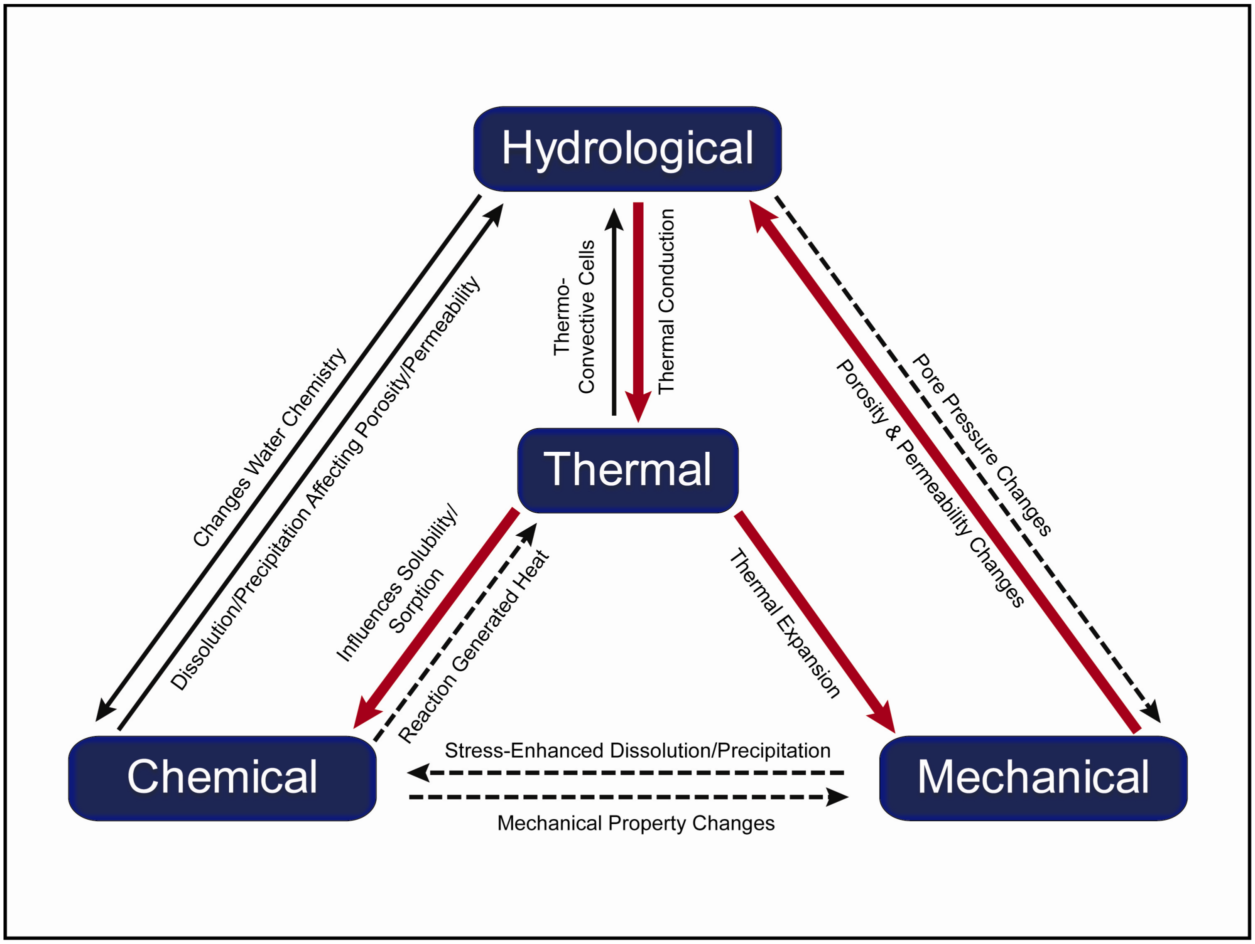

Figure 2-4. Conceptualization of Thermal-Hydrological-Mechanical-Chemical Interactions for Crystalline Host Rocks

2.3.2 Geochemical Processes

Crystalline rocks, such as granite and gneiss, are considered to have properties (e.g., high sorption and low dissolution) beneficial to repository performance. Elevated temperature in the near field resulting from waste emplacement could affect several geochemical processes as indicated in Figure 2-4, including radionuclide solubility and sorption and colloid stability. Near-field water chemistry also could change with temperature, which would affect waste container corrosion and waste form degradation. Mineral dissolution/precipitation occurring in the near field may change the hydraulic conductivity of the host rock (OECD/NEA, 2003), whereas water chemistry may change due to flow of groundwater with different composition.

Studies of natural hydrothermal alteration of granitic rocks show that dissolution of the silicate minerals potassium feldspar and plagioclase, which are the dominant phases in granite, could occur, accompanied by precipitation of quartz, clay minerals (mainly illites and smectites), and carbonates (calcite and dolomite) (Fritz, et al., 2010). However, the solubility and dissolution rate of silicate minerals at temperatures below about 100 °C [212 °F] are sufficiently low such that significant alteration of the crystalline host rock is unlikely at those temperatures. Numerical modeling by Fritz, et al. (2010) indicated that in the temperature range of 60 to 160 °C [140 to 320 °F], alteration of silicate minerals in the granitic rock played only a minor role in the short-term evolution of porosity. Carbonate minerals, which are minor phases in the unaltered granite, controlled the evolution of the porosity and permeability and are thus important to the long-term evolution of the system during the thermal period. The role of carbonate minerals is explained by higher kinetic rates for dissolution/precipitation of carbonates compared to that of silicates. Thus, in crystalline host rock repositories, the thermal effect on silicate dissolution/precipitation could be neglected as a first approximation, but carbonate dissolution/precipitation that could affect host rock porosity/permeability and radionuclide sorption/transport should be considered.

2.3.3 Geomechanical Processes

As discussed for argillaceous rocks in Section 2.1.3, crystalline rocks may deform in response to (i) excavation; (ii) heating due to radioactive decay of nuclear waste; (iii) change in internal fluid pressure due to drainage or pressurization; or (iv) other occurrences that affect rock stress. The deformation could be elastic and, therefore, fully reversible, or it could be inelastic. Inelastic deformations may occur when new cracks form or when existing cracks experience slip, opening, or closing. Therefore, inelastic deformation could result in coalescence of small cracks to form spatially persistent or connected fractures that may constitute paths for faster fluid flow. Additionally, inelastic deformation could result in partial closure and disconnection of previously connected fractures, thereby disrupting some existing through-going flow paths. Inelastic deformation also could cause rock blocks to detach from the roof of underground openings or could increase ground support loading.

Crystalline rocks contrast with argillaceous rocks in several ways that can help explain the nature of coupling among geomechanical and hydrological processes in the two rock types. First, unlike argillaceous rocks, crystalline rocks do not contain any appreciable amount of clay minerals or other constituents that may swell or shrink due to a water content gain or loss. Therefore, a change in suction is not likely to cause any appreciable deformation in crystalline rock. Suction changes in crystalline rock could have hydrological implications but are not likely to have any appreciable mechanical effect.

Second, in crystalline rocks, water is stored in and flows through microcracks and fractures. In contrast, water in argillaceous rocks is stored in and flows through pores, although water flow could be aided by any fractures that are sufficiently connected to provide enhanced drainage paths to pore water. Because of this difference between argillaceous and crystalline rocks, the hydrological effects of an excavation in crystalline rock differ from the effects in argillaceous rock. For both rock types, stress change due to an excavation and drainage at the excavation boundary could result in changes in water pressure and flow. In crystalline rocks, the effect of excavation on water flow is greater than the effect on water pressure. Furthermore, rapid decay of any water pressure change (e.g., Alonso, et al., 2005) because of the high conductivity of fractures will interfere with water pressure buildup due to stress change. Therefore, the hydrological effects of an excavation in crystalline rock are not likely to result in a water pressure change large enough to affect rock deformation. In contrast, an excavation in argillaceous rock could have immediate and appreciable effects on pore water pressure within the influence zone but only a delayed effect on water flow as the excess pore pressure decays slowly.

Based on the understanding of potential mechanical and hydrological processes in crystalline rock described in the foregoing paragraphs, stress change due to excavation could affect water pressure and flow; deformations could result in fracturing and, therefore, changes in porosity and permeability. However, the hydrological processes are not likely to have any appreciable effects on deformation. Potential thermal effects could be surmised similarly based on the expectation that free-draining fractures would interfere with water pressure buildup. However, suppressed thermal expansion of pore water or water in unconnected microcracks could result in water pressure buildup large enough to affect fracturing. If the contribution of such fracturing is small and, therefore, negligible, then potential hydrological effects on deformation can be considered negligible. For such a case, TM modeling need not be coupled with hydrological modeling to estimate the effects of deformations due to excavation or thermal loading in crystalline rock.

For example, Sobolik, et al. (2004) described an analysis to predict the effects of a tunnel excavation (FEBEX tunnel) for a heated drift test at the Grimsel Test Site in Switzerland. The analysis consists of (i) separate mechanical modeling to calculate stress change and deformations due to excavation and (ii) separate hydrological modeling to calculate water pressure and flow. The mechanical modeling included calculation of porosity and permeability changes due to the excavation, and the changes were applied as time-dependent input to the hydrological model. However, information Sobolik, et al. (2004) provided does not indicate whether the effects of stress change on water pressure were included in the hydrological model. A comparison of the calculated results with the corresponding measured response is inconclusive regarding adequacy of the modeling approach.

As a result, additional studies, such as sensitivity analyses or comparison of calculated and measured responses for controlled *in-situ* tests, will help evaluate whether TM modeling of the effects of excavation or thermal loading in crystalline rock should be coupled with hydrological modeling. Although the mechanical changes (such as stress change or fracturing) due to an excavation in crystalline rock could affect hydrological processes, the potential hydrological changes are unlikely to have any appreciable mechanical effects.

2.4 Coupled Processes in Salt

Salt formation (e.g., bedded salt, salt domes) is considered for a host medium because of its extremely low permeability, leading to practically very low groundwater flow conditions (IAEA, 2003). Thus, significant water entry into the repository is not envisioned, and transport of radionuclides away from the repository is limited to diffusion. However, there is potential for limited radionuclide transport from mobilized fluid inclusions in salt during the thermal phase. Salt rocks may deform in response to excavation, heating due to radioactive decay of nuclear waste, or other occurrences that affect rock stress. Based on a literature review, it can be concluded that salt deformation is time dependent and controlled by a creep rate that increases with temperature and deviatoric stress magnitude (Winterle, et al., 2011). This deformation may lead to creation of new fractures or enhance existing fractures, thus providing fast flow paths for radionuclide transport. Due to usually low permeability in salt formations, gas produced by microbial activities or chemical reactions may result in fracturing and enhanced permeability, if gas pore pressure exceeds the lithostatic pressure.

Site selection criteria for salt domes and bedded salt deposits generally include the avoidance of pockets of brine that may migrate under thermally perturbed conditions or salt zones with high potential for dissolution. Water in salt beds occurs naturally as fluid inclusions or brine pockets within void spaces, and at a smaller scale within the interstitial space between salt crystals. Fluid flow through such media is necessarily constrained to the interconnected porosity. In undisturbed formations, some water may be as old as the salt formation itself, having been trapped within the impermeable salt body as it formed. In a system perturbed by excavation and heat, however, porosity can easily evolve as salt crystals dissolve and recrystallize and changes in stress cause fractures that may interconnect pore spaces. In disturbed salt formations, mechanical fracturing (accompanied with salt damage, creep, and self-healing) and permeability dynamically evolve in time (Beauheim and Roberts, 2002).

The near-field disturbed zone is generally conceptualized to be limited in extent and to eventually heal to a state approaching *in-situ* permeability as the creep processes cause openings and fractures to gradually close. The period in which the near field remains in a disturbed condition is highly uncertain, depending on THMC processes and heat load, but could certainly persist for several thousand years.

In salt repositories, backfill consisting of crushed salt is expected to creep and recrystallize, becoming a part of the surrounding salt mass and completely sealing the openings. Elevated temperatures may influence the rate of salt creep in the surrounding rock, alter the chemical composition of minerals and waters or brines in the system, and may lead to cracking of the seals in the salt formation. Thermal perturbation also may have favorable effects in salt—the creep rate and thus the healing/sealing rate of the damage zone and crushed salt backfill increase with increasing temperature.

Coupled processes that may occur during the evolution of the damaged zone around excavations are described in the literature (Hansen and Leigh, 2011; Tsang, et al., 2005). The Wallner, et al. (2007) evaluation of THM evolution of the EDZ and backfill highlighted some issues, such as (i) the extent of brine migration toward waste packages, (ii) the spatial extent of the near field, and (iii) the length of time for the system (both the disturbed zone and backfilled seals) to return to natural hydrologic and geomechanical conditions.

Coupled processes in salt determine the amount of water available for corrosion processes. In salt formations, the overall availability of accessible water (brine) may be very limited compared to other porous, saturated geological media. Less information is available about corrosion of a metal encased in salt rocks. The main uncertainties in this respect are (i) the mobility and amount of water in the host salt rock that would be able to contact the metal and (ii) if the availability of liquid water is very limited, how the scarcity of water in the vicinity of a container would affect the corrosion rate in a repository setting.

Based on current staff understanding, the interaction of THMC processes for salt formation is conceptualized in Figure 2-5. The dominant linkages include (i) TM coupling that determines the creep rate that, in turn, causes a change in porosity and permeability; (ii) TC coupling that determines the temperature-dependent solubility and sorption properties of the formation; and (iii) TH coupling that determines the temperature-dependent fluid density and viscosity properties.

2.4.1 Thermohydrological Processes

Thermal perturbation by waste emplacement may alter the flow regime (IAEA, 2003). High thermal conductivity of salt deposits results in relatively lower temperatures compared to other host media. Thermal gradients induced by waste heat can cause various types of geochemical perturbations that could affect the flow regime. For example, solubility will increase slightly on the heated side of a brine pocket, resulting in dissolution on the hot side and precipitation on the cool side of the brine pocket that causes the brine to gradually migrate toward the heat source.

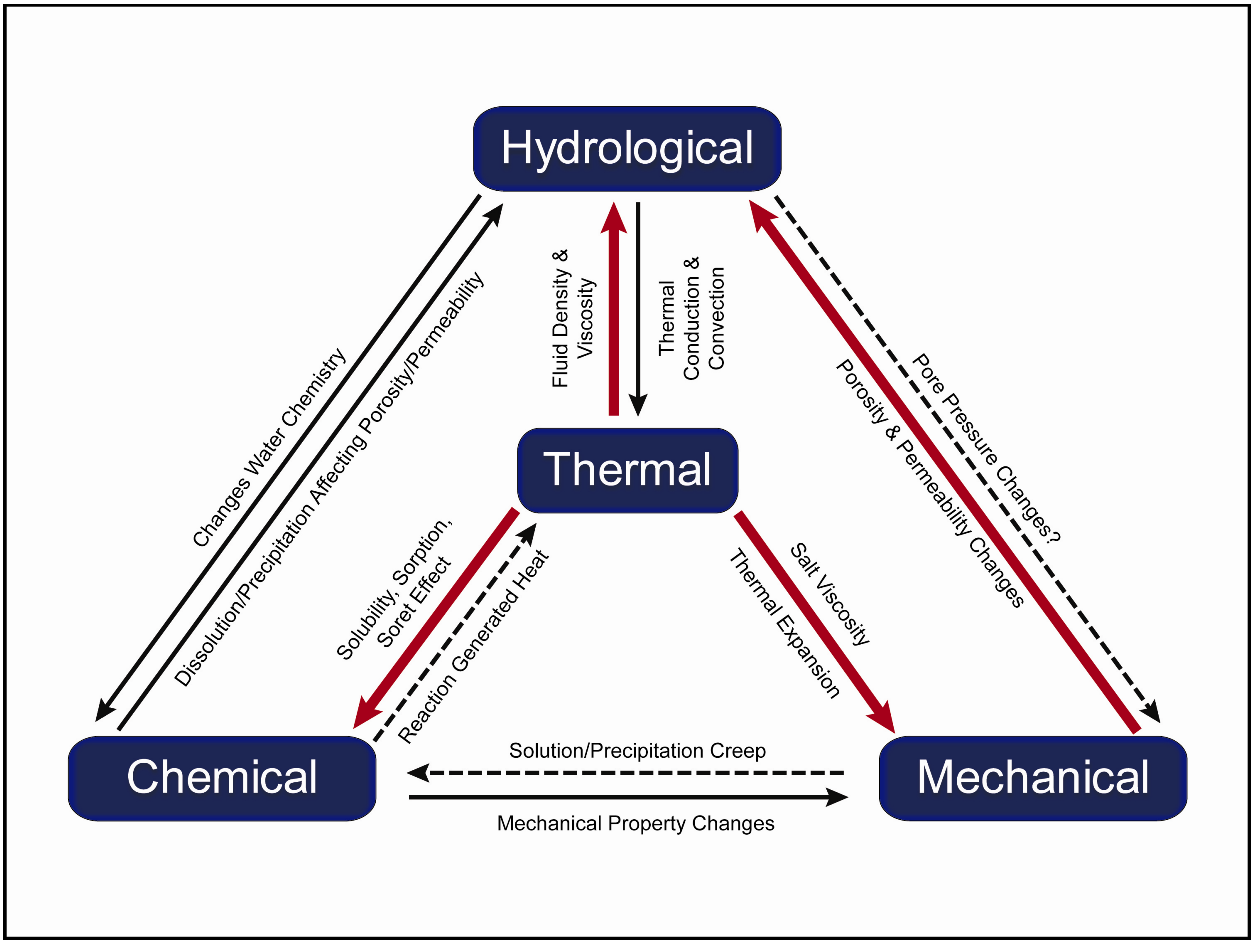

Figure 2-5. Conceptualization of Thermal-Hydrological-Mechanical-Chemical Interactions for Salt Rocks

Hansen and Leigh (2011) cite several examples of *in-situ* experiments in which such brine migration toward the heat source was observed. Temperature gradients could also cause evaporation and movement of water vapor within the near-field disturbed zone. Temperature gradients could result in thermally induced brine flow or two-phase flow. For example, temperature increases around waste located at the edges of the disposal chambers could cause evaporation of water entering from the excavated disturbed zone. This water vapor would condense in cooler areas in the emplacement chambers, including potentially condensing on cooler waste packages and contributing to brine formation, corrosion, and gas generation.

Studies have shown that excavation results in a damage zone of microfractures within a few centimeters [1 cm = 0.39 in] which results in enhanced permeability and the coalescence of fractures in the excavation damaged zone (Winterle et al., 2011). This could provide a pathway for fluid migration. Permeability within the disturbed zone could increase by three to seven orders of magnitude in response to the dilation (Hansen, 2003; Rath, et al., 2000).

Backfilling after emplacement of waste can help return the system to natural conditions faster than if no backfill is used by reducing the open volume that must be filled by rock wall deformation. The rate at which the salt system returns to natural conditions is uncertain and has been the focus of many laboratory and field experiments (e.g., Bechthold and Hansen, 2003). If crushed salt is used as a backfill, the hydrological regime in the near field will be influenced by the range of porosity and hydraulic conductivity of the backfill, which are in turn dependent on the particle size distribution of the crushed salt. The added effects of heating and subsequent cooling result in stress changes that may lead to new fracturing, or the opening existing fractures, depending on formation properties.

During the operational period of a repository, any accessible brine will tend to migrate down the stress gradient and evaporate into the ventilation air. The reconsolidation process, because of salt creep during postclosure, is expected to significantly limit brine flow to the waste disposal areas once the healing is complete. However, there is uncertainty regarding the heterogeneity of the creep process and this, in turn, could result in some repository locations that could experience brine flow for extended periods. The amount of brine flow is dependent on the TH and THM/HM coupled processes in the near field. This potential for brine flow should be evaluated in detail in terms of its effect on flow and transport of radionuclides.

2.4.2 Geochemical Processes

The effect of elevated temperature due to waste emplacement on geochemical processes in a salt host rock repository is likely to be greater than in an argillite or crystalline host rock repository. The greater effect is due to the much higher solubility of minerals present in a salt repository compared to those in argillite and crystalline host rocks and to the stronger temperature effect on the solubility of salt minerals. Brines that form in a salt repository likely will be corrosive to waste containers, and higher temperatures would increase the corrosion rate. Higher temperature in the near field also could increase the degradation rate of the waste form and other engineered materials (e.g., seals), increase radionuclide solubilities, and decrease radionuclide sorption (Figure 2-5). Mineral dissolution and precipitation could alter (i) the hydrological properties of the salt host rock and (ii) pore water composition resulting in changes to the near-field water chemistry. In addition, changes in the mineralogical composition of the salt host rock could significantly alter its mechanical properties.

Temperature can affect brine chemistry in another manner. Gases such as H_2S, HCl, CO_2, and SO_2 can be released from natural salt upon heating (Uerpmann and Jockwer, 1982; Pederson, 1984; Jockwer, 1984). Impurities within the salt apparently contain one or more of these thermally unstable, acidic components. These components can volatilize during heating and increase the alkalinity of residual brines. In an open repository system, the acidic gases would escape and leave potentially alkaline-producing salt. However, in a sealed system the gases may accumulate near the waste containers and eventually form acidic brines.

2.4.3 Geomechanical Processes

Salt rocks may deform in response to excavation, heating due to radioactive decay of nuclear waste, or other occurrences that affect rock stress. As reviewed in more detail by Winterle, et al., (2011, Chapter 2), salt deformation is time dependent and controlled by a creep rate that increases with temperature and deviatoric stress magnitude. An excavation in salt increases deviatoric stress within the influence zone of the excavation. The rock deforms to restore equilibrium at a rate that depends on the temperature and magnitude of stress change, even if the stress change is small. Also, the rock deforms in a time-dependent manner to adjust to a new equilibrium state after an increase in deviatoric stress due to heating from disposed nuclear waste. As discussed in Sections 2.1.3 and 2.3.3, thermal loads could cause an increase in deviatoric stress because of suppressed thermal expansion due to nonuniform temperature distributions. Therefore, thermal effects on deformation can arise due to the effects of temperature on salt creep rate and the effects of suppressed thermal expansion on rock stress.

The result of salt rock deformation depends on whether the prevailing stress states during the deformation favor dilation or compaction. Salt dilation (inelastic increase in volume) consists of growth and opening of microcracks and pores, increases porosity and permeability and decreases stiffness and load-bearing capacity, and is driven by stress states characterized by a high ratio of deviatoric stress to confining stress. In contrast, salt compaction (non-recoverable decrease in volume) consists of closure of microcracks and pores, decreases porosity and permeability and increases stiffness and load-bearing capacity, and is driven by stress states characterized by a low ratio of deviatoric stress to confining stress. Dilation is associated with damage, whereas compaction is associated with healing. Laboratory studies of the dilation and compaction tendencies of rock salt have helped define a surface in stress space referred to as the dilatancy boundary, which distinguishes between stress states that favor dilation and stress states that favor compaction (e.g., Hunsche and Hampel, 1999; Hansen, 2003; Schulze, 2007; Alkan, et al., 2007). Stress states within the dilatancy boundary favor healing, whereas stress states outside the dilatancy boundary favor damage. In addition, rheological contrasts due to material nonhomogeneity or temperature gradients can affect the deformation mode [i.e., damage versus healing, as detailed in Winterle, et al. (2011, Chapter 2)].

Salt rock deformations need to be evaluated to assess potential effects on fluid flow or the environment and loading of waste containers. Dilation could result in zones of microcracks or dilated pores that may coalesce to form faster flow paths for fluids. Conversely, healing could close existing cracks and pores, thereby disrupting existing flow paths. Also, deformation could result in external pressure on waste containers, if the host rock converges into the openings and contacts the containers. Furthermore, a container could sink into the floor rock through progressive mobilization of heated salt at the container base and the mobilized salt rising to “condense” above the container, thereby increasing downward pressure on the container. The process could result in the container being submerged in the salt or exiting from the salt formation to an underlying nonsalt geologic material.

Mechanical modeling to evaluate salt rock deformations may not need to be coupled with hydrological modeling. Although deformation can affect fluid flow as described previously, there does not appear to be any mechanism for an appreciable hydrological effect on deformation. As reviewed in more detail in Winterle, et al. (2011, Chapter 3), water likely occurs in salt rock as isolated inclusions that may drain if a flow path occurs but lack the continuity necessary to develop water pressure that can affect rock deformation. Nonsalt layers or zones within the salt rock could potentially contain water and develop sufficient water pressure to affect deformation. Therefore, while the basic mechanical modeling may not need to be coupled with hydrological modeling, potential effects of water pressure in nonsalt layers need to be evaluated. Furthermore, rock salt subjected to stress conditions within the dilatancy boundary may, in addition to mechanical compaction, undergo geochemical healing through a mass transfer process, such as solution and reprecipitation or crystallization (e.g., Hansen, 2003; Lux and Eberth, 2007; Schulze, 2007). Such geochemical healing could increase mechanical strength and stiffness, thereby affecting subsequent evolution of stress and deformation. However, although the effects of geochemical healing on deformation may need to be accounted for in mechanical modeling, there are considerable uncertainties regarding quantification of geochemical healing.

2.5 Summary

Geologic media broadly categorized into argillaceous, crystalline, and salt formations are being considered as host rocks for radioactive waste disposal. The host media and buffer/backfill materials are intended to isolate wastes from the near-surface environment; maintain geochemical, hydrogeological, and geomechanical environments favorable to the preservation and performance of the EBS; and act as a natural barrier restricting water access to the wastes and the migration of mobilized radionuclides. However, THMC coupled processes associated with the heat load the emplaced radioactive waste imposes on the geologic media and HMC coupled processes during the postthermal period can affect the ability of the host media and buffer/backfill materials to isolate the waste and mitigate the migration of radionuclides. Understanding these couplings of processes is essential for a reliable assessment of repository performance and for the evaluation of the safety case.

Argillaceous clay-rich formations, such as plastic and indurated clays, shales, and mudstone, are considered as potential repository host rocks because of their favorable hydrologic (low permeability), chemical (low diffusion coefficient, high retention capacity for radionuclides), and mechanical properties (capability to self-seal fractures induced by tunnel excavation). Low permeability and porosity of argillaceous formations result in long durations for drying and resaturation of the host rock. Possible geochemical effects include (i) transformation of smectite to illite that could lead to an embrittlement and a partial or total loss of swelling capacity; (ii) dissolution/precipitation reactions and clay mineral alteration that could change the hydraulic conductivity of the argillite; (iii) changes in the pore water chemistry that could affect radionuclide solubility and sorption, waste package corrosion, and waste form degradation; (iv) modification of the ion-exchange, hydration, and swelling behavior of the clay minerals; and (v) alteration of clay colloid stability. Degradation of organic material also could occur and lead to production of CO_2 or monocarboxylic acids, which, in turn, could (i) change the pore water pH and ionic strength; (ii) dissolve carbonate minerals; and (iii) change ion-exchange equilibria, clay surface properties, and radionuclide speciation and sorption. Temperature could have a significant effect on clay mineral/colloid stability and radionuclide solubility and sorption, whereas chemical processes, such as dissolution/precipitation reactions and clay alteration, could modify the hydrologic properties of the argillite host rock. On the other hand, water chemistry in the near field could be changed by flow of groundwater with different composition. Rock fracturing due to excavation, thermal loading, or drying shrinkage could affect water flow and pore pressure dissipation because of the enhanced hydraulic conductivity. Furthermore, a change in pore water pressure due to drainage, imbibitions, or thermal expansion could affect fracturing or fracture healing. Therefore, estimating damage-zone evolution in argillaceous rock entails a coupled THM modeling.

Based on current staff understanding, the dominant THMC processes for argillaceous formations include the (i) TH coupling that refers to the influence of thermal load on the rate of saturation and desaturation processes; (ii) TC coupling that refers to the temperature-dependent chemical characteristics such as solubility and sorption coefficients and clay mineral and colloid stability; (iii) TM coupling that influences the rate of swelling (thermal expansion); and (iv) HM coupling that indicates the influence of saturation on development of pore pressures that influence the swelling process.

Bentonite or a bentonite–sand mixture is proposed as a buffer and backfill material in a number of countries. The hydrological (low hydraulic conductivity), geochemical (very low diffusion, high sorption, good colloid and microbial filtration capability), and mechanical (high swelling potential enables self-sealing of openings) properties of bentonite make it a favorable buffer/backfill material between the waste packages and host formation. Drying and resaturation rates are controlled by thermohydrological properties and buffer design. These processes are very slow because of low permeability and presence of a thermal gradient. Chemical or mineralogical changes in the bentonite buffer/backfill could occur due to heating in the near field. The main thermal-chemical effect on bentonite may be heat-induced transformation of montmorillonite to either beidellite or illite, which could lead to embrittlement, a partial or total loss of swelling capacity, and an increase in hydraulic conductivity of the clay material. Higher temperatures also could (i) enhance dissolution/precipitation reactions (e.g., involving silica or calcite) that could alter the hydraulic conductivity and possibly create preferential flow paths in the bentonite buffer/backfill; (ii) change pore water chemistry that could affect radionuclide solubility and sorption, waste package corrosion, and waste form degradation; (iii) modify the ion-exchange, hydration, and swelling behavior of the clay minerals; and (iv) alter clay colloid stability. In addition, degradation of organic material and production of CO_2 or monocarboxylic acids could be enhanced, which, in turn, could (i) change the pore water pH and ionic strength; (ii) dissolve carbonate minerals; and (iii) change ion-exchange equilibria, clay surface properties, and radionuclide speciation and sorption. Simultaneous temperature and water-saturation gradients in a buffer could result in cracking due to desiccation or crack healing due to swelling. Also, frictional resistance at buffer vertical walls may result in cracking due to loss of vertical confinement. If cracks in the buffer are subjected to high water-flow velocities, buffer materials could erode internally. Therefore, estimating buffer damage due to cracking and internal erosion entails a coupled THM modeling.

Based on current staff understanding, the dominant THMC processes for buffer/backfill include (i) the TH processes that affects the spatial and temporal distribution of the saturation during the drying and rewetting of buffer during the initial postclosure period; (ii) the degree of swelling that is controlled by the HM coupling with a strong impact of the thermal pulse; (iii) the THC/TC coupling that determines the chemical composition of the buffer, which impacts the retardation capabilities of the buffer (sorption, solubility, colloid properties); and (iv) the TMC coupling that could change mechanical properties for above-boiling conditions.

Cementitious materials are major components of engineered barriers or structures in most LLW, ILW, and transuranic TRU waste geologic disposal repositories and in some HLW repository concepts. These materials are used in repository vaults, floors, tunnel linings and plugs, waste conditioning matrices, and backfill. Because of the alkaline pH of cement pore waters, interaction with crystalline and argillite host rocks and with clay buffer/backfill is an important geochemical process that needs to be considered in performance assessments. The alkaline pH of cement pore waters could alter the host rock mineralogy and buffer/backfill properties. Dissolution and precipitation processes could occur and result in porosity/permeability changes that alter groundwater/gas flow pathways in the host rock and buffer/backfill. For example, dissolved carbonate ions in solution are known to react with calcium in the cement to form calcite and seal the pores or fractures in the cementitious material or in the adjacent rock. Interaction of groundwater with cementitious materials also could change the water chemistry and affect radionuclide solubility and sorption. Vitrified waste form dissolution is expected to be faster at higher pH, although spent fuel dissolution rate likely will be unaffected by alkaline solutions.

Crystalline rocks, such as granite and gneiss, are considered for their hydrogeological (low permeability in unfractured rocks), mechanical (high strength), and geochemical characteristics (high sorption and low dissolution) that are beneficial to repository performance (Table 2-1). The flow regime in crystalline rocks is governed by the extent of fracture connectivity and presence of structural features such as faults. Elevated temperature in the near field resulting from waste emplacement could affect several geochemical processes, including radionuclide solubility and sorption and colloid stability. Near-field water chemistry also could change with temperature, which would affect waste container corrosion and waste form degradation. Mineral dissolution/precipitation occurring in the near field may change the hydraulic conductivity of the host rock, whereas water chemistry may change due to flow of groundwater with different composition. Stress change due to excavation or thermal loading could cause rock fracturing and increase in porosity and permeability and could directly affect water pressure and flow. However, the hydrological processes are not likely to have any appreciable effects on rock deformation. Therefore, damage-zone evolution in crystalline rock could be estimated using TM modeling alone. TM modeling need not be coupled with hydrological modeling, if the effects of water pressure changes on deformation and the effects of fracturing on porosity and permeability are accounted for in the TM and hydrological models.

Based on current staff understanding, the dominant THMC processes for crystalline rocks include (i) TM coupling that influences the thermal deformations which, in turn, could lead to changes in permeability and porosity; (ii) TH coupling that influences the thermal conduction processes; and (iii) TC coupling that influences the solubility and sorption properties of the host rock.

Salt is considered for a host medium because of its extremely low permeability, leading to practically very low groundwater flow; this implies there will be less potential for radionuclide transport. Temperature gradients could result in thermally induced brine flow or two-phase flow. Condensation on cooler waste containers in the chambers could contribute to brine formation, corrosion, and gas generation. Brines that form in a salt repository likely will be corrosive to waste containers, and higher temperatures would increase the corrosion rate. Higher temperature in the near field also could increase the degradation rate of the waste form and other engineered materials (e.g., seals), increase radionuclide solubilities, and decrease radionuclide sorption. On the other hand, mineral dissolution and precipitation could alter the hydrological properties of the salt host rock and flow of groundwater with different composition could change the near-field water chemistry. In addition, changes in the mineralogical composition of the salt host rock could significantly alter its mechanical properties. Gases such as H_2S, HCl, CO_2, and SO_2 also can be released from natural salt upon heating. In an open repository system, the acidic gases would escape and leave potentially alkaline-producing salt. However, in a sealed system the gases may accumulate near the waste containers and eventually form acidic brines. Deformations need to be evaluated to estimate rock damage or healing that may affect the evolution of fluid flow paths and the environment and loading of waste containers. Mechanical modeling to evaluate deformations need not be coupled with hydrological modeling, but the effects of water pressure in nonsalt layers or zones need to be evaluated. The effects of geochemical healing on mechanical behavior could be important but include considerable uncertainties.

Based on current staff understanding, the dominant THMC processes for salt formations include (i) TM coupling that determines the creep rate which, in turn, causes a change in porosity and permeability; (ii) TC coupling that determines the temperature-dependent solubility and sorption properties of the formation; and (iii) TH coupling that determines the temperature-dependent fluid density and viscosity properties.

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3 REPRESENTATION OF COUPLED PROCESSES IN NUMERICAL MODELS

3.1 Coupled Processes

Two-way interactions and feedback mechanisms among Thermal-Hydrological-Mechanical-Chemical (THMC) processes for a generic host rock are shown in a quad-linear diagram in Figure 1-1. For example, porosity and permeability (and hence, flow rates and flow paths) of a host rock may be altered due to combined effects of mechanical processes (e.g., stress-induced fracturing, inelastic or elastic deformations, self-healing), chemical reactions (e.g., dissolution, precipitations), and thermal processes (e.g., thermal expansion of the host rock and resultant fracturing). Chemical reactions in the host rock could be affected by altered water-flux and radionuclide mass-flux rates along modified flow paths; spatiotemporal variations in thermal conductivity and temperature distributions across the host rock; and mechanically altered size, surface properties, and distribution of reactive surfaces (e.g., sites for irreversible sorption of radionuclides). Changes in flow rates and flow paths could affect the rate of energy transfer and effective stress distributions in the host rock. Spatiotemporal variations in temperature distribution could result in mechanical instabilities in the host rock, changes in advective flow rates and flow paths, and phase changes.

The relative strength and importance of interactions among THMC processes would depend on physical, hydrological, mechanical, and chemical properties of a host rock; existing flow conditions; and specific engineering applications to be undertaken. The review in the subsequent sections focuses on capabilities and suitability of selected numerical models to simulate THMC processes in different geological media for deep disposal of high-level nuclear waste.

3.2 Process-Level Numerical Models for Thermal-Hydrological-Mechanical-Chemical Simulations

Table 3-1 lists and compares capabilities of several process-level numerical models commonly used in the United States for simulating various combinations of coupled THMC processes in different geological media. Although various combinations of THC modeling components, through built-in or external couplings, have been well documented and used for simulating laboratory- and field-scale flow and transport problems, their integration with the M component is currently in progress. Among the simulation capabilities listed in Table 3-1, we considered the following capabilities to be crucial for simulating THMC processes: (i) nonisothermal flows in three-dimensional and variably saturated fractured, porous, or fractured-porous flow domains and (ii) spatiotemporal changes in porosity and permeability of the host rock in response to mechanical, chemical, and thermal stresses. Based on these modeling features, TOUGHREACT-FLAC3D, STOMP, and PFLOTRAN appear to have more mature simulation capabilities than the others listed in Table 3-1. Specifically, the current version of the coupled TOUGHREACT-FLAC3D is the only numerical model with built-in capabilities for three-dimensional THMC simulations in a variably saturated fractured porous host rock with spatiotemporal changes in its porosity and permeability. In its current version, TOUGHREACT is externally linked to a geomechanics code, known as FLAC3D (Rutqvist and Tsang, 2003; Javeri and Baltes, 2008).

Table 3-1. Numerical Models Evaluated for Representing Thermal-Hydrological-Mechanical-Chemical Processes in Geological Media

Modeling Features	*xFlo*	STOMP	HYDRUS	TOUGHREACT -FLAC3D	CONNECT FLOW	PFLOTRAN	MODFLOW MT3DMS	GWB X1t, X2t	PHREEQC	ABAQUS	FLAC, FLAC3D	UDEC, 3DEC
Dimension	3D	3D	3D	3D	3D	3D	3D	1D, 2D	1D RT	3D	3D	3D
C/D	C	C	C	C	D	C	C	C	C	C	C	D
F, P, FP, DP	F, P, FP	F, P, FP	F, P, FP	F, P, FP	F, P	F, P, FP	P	F, P, DP	DP	FP	P	F
SP, MP, MC	MP, MC	MP, MC	MP, MC	MP, MC	MP	MP, MC	SP, MC	SP, MC	SP, MC	SP	SP	SP
Thermal	Non-iso	Non-iso	Non-iso	Non-iso	Non-iso	Non-iso	Iso	Non-iso	Non-iso	Non-iso	Non-iso	Non-iso
Phases	Aq, G	Aq, G, I, H	Aq, G	Aq, G, I, H	Aq, G	Aq, G	Aq, G	Aq, G	Aq	Aq	Aq	Aq
Freezing Soil	N	Y	IP	Y	N	IP	N	N	N	N	N	N
Chemistry	N	Y	Y	Y	N	Y	N	Y	Y	N	N	N
Reaction	None	E/K, SC, Dec, P/D	E/K, SC, R, CE Dec, P/D	E/K, SC, R, CE, Ex Dec, P/D, A/B	SLR, Dec	E/K, P/D, IE, GS	coupled with PHREEQC	E/K, P/D, SR	E/K, SC, Dec, P/D, CE, IE			
Perm/Por Changes	N	Y	Y (in 1D only)	Y	N	Y	N	Y	N	Y	N	N
GeoMech	N	IP	N	Y (E)	Y (B)	N	N	N	N	Y	Y	Y
Colloids	N	Y	Y	Y	N	N	N	N	N	N	N	N
Gridding	U	U	U	U	U	U	S	S	S	U	U	U
Developed by	CNWRA/ NRC	Pacific Northwest National Laboratory	United States Salinity Laboratory	Lawrence Berkeley National Laboratory	Serco's Technical Consulting Services	Los Alamos National Laboratory	USGS	University of Illinois	USGS	Dassault Systemes Simulia Corp.	Itasca International	Itasca International

RT: Reactive Transport
C/D: Continuous vs. Discrete
F, P, FP, DP: Fracture, Porous, Fracture-Porous, Dual Porosity
SP, MP, MC: Single-Phase only, Multi-Phase, Multi-Component
Non-Iso, Iso: Non-Isothermal, Isothermal
Aq, G, H, I: Aqueous, Gas, Hydrate, Ice
E/K: Equilibrium/Kinetic Reactions; SC: Surface Complexation; Dec: Decay; P/D: Precipitation/Dissolution; R: Redox Reactions; CE: Cation-Exchange; A/B: Acid-Base; Ex: Exsolution; SLR: Solubility-Limited Reactions; IE: Ion-Exchange; GS: Gaseous-Speciation Reactions; SR: Speciation Reactions;
Perm/Por Changes: Temporal Changes in Permeability and Porosity
GeoMech: Geomechanical Component; (E): Externally Coupled; (B): Built In
U: Unstructured; S: Structured
N, Y, IP: No, Yes, In Progress
CNWRA: Center for Nuclear Waste Regulatory Analyses
NRC: U.S. Nuclear Regulatory Commission
USGS: U.S. Geological Survey

On the other hand, the current version of STOMP is suitable for THC simulations in three-dimensional, dynamically evolving (with spatiotemporal changes in porosity and permeability), fractured porous domains, and its integration with a geomechanics component is reportedly in progress. Similarly, the current version of PFLOTRAN is also limited to THC simulations in dynamically evolving, fractured porous domains.

As discussed previously, TOUGHREACT is externally coupled with a stand-alone geomechanics code (FLAC3D), which is suitable for simulating large displacements and strains, nonlinear material behaviors, and unstable systems. However, other stand-alone geomechanics models with different modeling strengths and capabilities could also be externally linked to THC models for THMC simulations. Among such geomechanics codes, ABAQUS is suitable for linear and nonlinear structural analysis under static and dynamic loadings and geotechnical interactions. ABAQUS has been extensively used in the Swedish nuclear waste program and in earlier DECOVALEX phases (Alonso, et al., 2005). However, such applications did not consider permeability change in the host rock in response to geomechanical processes (Rutqvist, et al., 2009). Another geomechanics code, UDEC/3DEC, is well suited for engineering problems involving jointed rock systems or assemblage of discrete rock blocks subjected to quasi-static and dynamic conditions and has been used to assess a nuclear waste repository in Sweden (Lönnqvist, et al., 2010). For salt host rocks, SNL Sierra Mechanics, which was specifically developed for studying geomechanical processes in salt, could be linked to THC models (Hansen and Leigh, 2011).

In addition to the numerical models listed in Table 3-1, other process-level THMC models that are being used in Europe and Japan for evaluating the suitability of different geological media for waste disposal include the following:

- HM3D was used to simulate HM processes in granite rocks at the GTS Site in Switzerland (Kadiri, et al., 2002). HM3D encompasses externally linked RESOBLOK (flow domain geometry model), 3DEC (geomechanics model), and 3FLO (hydrology model).

- A coupling of ROCKFLOW/ROCKMECH was used to simulate THM processes in argillaceous clay in Germany (De Jonge, et al., 2004).

- ROCMAS was used to study coupled THM responses at FEBEX at the Grimsel Test Site in Switzerland (Rutqvist and Tsang, 2004).

- FRACOD was used to simulate TH processes at the TSX tunnel of URL in Canada, the ZEDEX tunnel of the SKB Äspö Hard Rock Laboratory in Sweden, and the deposition tunnel in crystalline and sedimentary rocks in Japan (Stephannson, et al., 2008).

- COMSOL Multiphysics was used to simulate THMC processes across bentonite barriers in two- and three-dimensional hypothetical granitic host rocks (Olin, et al., 2008).

- THAMES, a coupled THM model, was applied in the DECOVALEX project and in the Japanese nuclear waste program (Chijimatsu, et al., 2005).

In the subsequent sections, THMC properties of argillaceous (and buffer), crystalline, and salt rocks will be summarized. Based on these properties, the relative strength and importance of THMC couplings for each host rock type will be identified and suitable numerical models from a pool of numerical models discussed in this section for simulating THMC processes in each host rock will be discussed.

3.2.1 Argillites and Buffer

As discussed in Section 2.1, argillites are characterized as low permeability and high capillary pressure flow media. Argillaceous clay can deform elastically (reversibly) or inelastically (permanently) under thermal, chemical, and mechanical stresses. Under saturated conditions, it can swell, creep, and behave plastically. Under dry conditions, however, it can shrink and become brittle. When argillaceous clay is saturated, its deformable nature could result in self-healing and sealing. Argillaceous clay has higher sorption capacity than salt or crystalline host rocks, and its mineral content could be altered (depending on the clay type) at elevated temperatures, especially at above-boiling conditions.

Flow conditions in low permeability argillaceous host rocks in the near-field zone could depend on (i) saturation-induced permeability, porosity, and mechanical stability alterations; (ii) thermal stress-induced mineral alterations and consequently mineral precipitation or dissolution; and (iii) alterations of reactive surfaces along flow paths. Thus, based on current staff understanding, THMC coupling at high temperatures or HM coupling in the absence of thermal stress would need to be strong in simulating near-field flow and transport in argillaceous clay. In THMC or HM couplings, the staff suggest that the TH module should be able to calculate the average pore pressure, temperature, and saturation and pass them to the M module. Based on this information, the M module would calculate the stress distribution and the resultant changes in porosity, permeability, and capillary pressures in the argillaceous host rock, similar to the HM coupling implemented in TOUGH-FLAC3D (Rutqvist and Tsang, 2003). Moreover, THMC coupling is expected to be strong in the buffer zone and in the disturbed zone, where the impacts of mechanical stress would be significant.

Because THMC and HM couplings could be important for argillaceous clay in the near field and THMC coupling would be important in the buffer zone around the damaged zone, TOUGHREACT-FLAC3D, RockFlow/RockMech, ABAQUS, COMSOL, and STOMP would be suitable numerical codes for such simulations. To the staff's knowledge, TOUGHREACT-FLAC3D coupling was used to study CO_2 injection into a saline aquifer in the North German basin (Hou, et al., 2010), but has not been used for studying deep geological disposal of high-level nuclear waste. Among the numerical codes listed in Table 3-1, TOUGH-FLAC3D (for THM simulations) and TOUGHREACT-FLAC3D (for THMC simulations) are the only simulators that can simulate porosity and permeability changes due to mineral clay swelling.

3.2.2 Crystalline Rocks

Crystalline rocks consist of massive fractured rock blocks. They exhibit two hydraulically distinct zones. Fractured zones are relatively high-conductivity zones, through which advective flow and transport would occur. The matrix zone is typically low permeable to impermeable and matrix diffusion could occur at fracture–matrix interfaces.

Mechanically altered fractures and joints in crystalline rocks determine flow paths and rates in saturated and unsaturated flow conditions. Because crystalline rocks exhibit medium thermal conductivity (Table 2-1), sufficiently high thermal stress could induce fracturing and, hence, additional fracture flow paths. In simulating flow and transport in crystalline rocks, combined effects of mechanical and thermal stresses need to be incorporated in the momentum equation (Watanabe, et al., 2009).

Based on current staff understanding, if the thermal load is significantly lower, HM coupling needs to be strong in simulating flow and transport in crystalline rocks. At higher thermal stresses, THM needs to be coupled strongly. THC coupling could be important: if the main fracture flow paths are narrow, flow rate in such fractures is low, which could allow sufficiently long water–fracture wall contact/reaction times, and if the water is oversaturated with chemical constituents such that precipitation could occur in narrow flow paths. However, in general, THC coupling would be less significant than THM coupling for nonisothermal flow and transport in fractured crystalline rocks.

Because THM or HM coupling would prevail for fracture flow and transport in crystalline rocks under saturated and unsaturated flow conditions, CONNECTFLOW, COMSOL, ABAQUS, UDEC/3DEC, and TOUGH-FLAC would be suitable numerical codes for such simulations.

3.2.3 Salt Rocks

As discussed in Section 2.4, salt rocks are characterized by very low porosity and permeability. However, if salt rock is disturbed (e.g., through excavations), large-scale visible fracturing can develop near the disturbed zone with, for example, reportedly four to seven orders of magnitude increases in permeability over a range of dilatant volumetric strain in the range of 0.5–4 percent (Rath, et al., 2000). Fracturing, and hence permeability development, in salt can be induced due to thermal stresses. If sufficient fluid–rock contact time occurs, chemical dissolution could also lead to permeability enhancement. However, fractures in salt may undergo self-healing, if fracture mass reloaded along the hydrostatic axis.

Fluid flow in salt is affected by hydrologic properties of the host rock (e.g., impurities, bedded evaporates, extent and rate of fracturing). In turn, fluid flow could affect mechanical fracturing because of salt damage, creep (viscoplastic deformation), and self-healing. Mechanical fracturing and fluid flow in salt evolve over time; hence, permeability is a spatially and temporally variant hydrologic property of a host rock (Beauheim and Roberts, 2002), which needs to be addressed in numerical simulations.

Laboratory experiments (Alkan, 2009) revealed that when the vertical stress exceeded the dilatancy stress threshold, porosity and permeability of the salt rock increased as the vertical stress increased. This observation suggests that in numerical simulations, permeability of the rock salt can be related to the normal stress or volumetric strain rate. Thus, empirical relations that relate rock salt permeability, *k,* to normal stress, σ_3 (Alkan, 2009), or volumetric strain, ε_γ (Pudewills, 2005), were developed for one-dimensional HM simulations.

As discussed previously, fracturing in salt may result from (i) mechanical processes (as pore pressure exceeds lithostatic pressure in low permeability domains and/or vertical stress exceeds the dilatancy stress threshold), (ii) thermal expansion of salt with high thermal conductivity, or (iii) dissolution (as the fractured regions are contacted by fluid). Thus, based on current staff understanding, THM and/or THC coupling needs to be strong under thermal stress; otherwise, HM coupling needs to be strong. In the absence of thermal stress, the C module would be relatively less important due to (i) the less sorptive nature of salt and (ii) the existence of limited volume of water and water–rock contact areas in self-healing fractures and low permeability flow pathways.

For salt, THM coupling would be crucial under thermal stress and HM coupling would be crucial when thermal stress is absent or weak; therefore, ABAQUS, TOUGH-FLAC, or SNL Sierra Mechanics would be suitable numerical codes for such simulations.

3.3 Development of In-House Code Capabilities

Development of in-house capability for modeling THM and THC numerical codes, rather than using existing codes from other institutions, has the advantage of increased flexibility to add and test options for addressing new modeling components and techniques. It also helps staff to develop a deeper understanding of the applicability and limitations of numerical simulations.

The U.S. Nuclear Regulatory Commission and the Center for Nuclear Waste Regulatory Analyses currently have a TH numerical code named *xFlo* (Painter, 2006). It is a multiphase, thermohydrologic, dual-continuum, flow and transport simulator (Table 3-1). The *xFlo* code adopted the TH routines of MULTIFLO™ (Painter, et al., 2001), but used object-oriented programming in a modular code structure. The full range of code capabilities has not been (software) validated since evolving from MULTIFLO. This will need to be addressed before initiating any in-house code development. Such codes would provide an independent means for testing and/or validating site-specific proposed conceptual models and computed numerical results.

Several options are available for creating THM and THC numerical codes. The options differ in level of difficulty and effort, but all would use *xFlo* as a starting point. These options are individually applicable to either a THM or a THC code.

1. Develop a fully integrated code that directly solves equations for all three processes, either THM or THC. This option also encompasses operator splitting techniques that simplify the governing equation for one or more of the processes, thus reducing the computational burden.

2. Modify the existing *xFlo* TH code to link on a timestep level with other existing codes, either geomechanical or geochemical. Examples for geomechanical processes include FLAC3D, ABAQUS, or 3DEC, and for geochemical processes include Geochemical Workbench X2t or GEM.

3. Modify the existing *xFlo* code to link on a simulation-period level with output from other existing codes (using the same other codes as listed in the second item above). The primary modification to *xFlo*, besides reading in new external files, would be to implement time dependency for parameters that may change due to geomechanical or geochemical processes.

The three options are listed in order of level of difficulty and effort, highest to lowest. The first option would likely require a full-time code custodian and supporting expertise in THMC processes. The second option significantly reduces the level of effort needed to develop THM or THC code, but would likely require some interactions with geomechanical or geochemical code producers. Some (small) changes to existing codes may be needed; thus, willingness on the part of the geomechanical or geochemical code developer would be required. The last listed option allows for a slightly smaller level of effort compared to the second option. Considering all three options, there may be a decrease in flexibility, and potentially accuracy, for the range of problems to address going from the first through third options. This is because there may be changes needed wholly within the geomechanical or geochemical codes that are beyond simple linking changes. The types of problems include instances where mechanical or chemical issues are prominently affected by TH processes.

There have been substantial efforts to develop centralized internationally recognized and quality-assured chemical thermodynamic databases, for example, the Nuclear Energy Agency Thermochemical Database and Nuclear Waste Management Organization Thermodynamics/Sorption database, among others. Such centralized and high-quality thermodynamic databases would be used to construct look-up tables and parameter sets for the aforementioned in-house coupled THC model.

3.4 Summary

Based on staff's current understanding, prevailing THMC processes in argillites, crystalline rocks, and salt were identified and suitable numerical models for simulating flow and transport in these media were proposed. Briefly, for argillites, THMC or HM couplings would be crucial in the near field and THMC coupling would be crucial in the buffer zone; therefore, TOUGHREACT-FLAC3D, RockFlow/RockMech, ABAQUS, COMSOL, and STOMP would be suitable numerical codes for such simulations. For crystalline rocks, THM or HM coupling would prevail; therefore, CONNECTFLOW, COMSOL, ABAQUS, UDEC/3DEC, and TOUGH-FLAC would be suitable numerical codes for such simulations. For salt, THM coupling under thermal stress and HM coupling in the absence of weak thermal stress would be crucial; therefore, ABAQUS, TOUGH-FLAC, or SNL Sierra Mechanics would be suitable numerical codes for such simulations. NRC and CNWRA currently have a TH numerical code -*xFlo*, which is a multiphase, thermohydrologic, dual-continuum flow and transport simulator. As an alternative to using existing codes, the *xFlo* model can potentially be improved by adding M or C modules for THM and THC simulations in the aforementioned rock types.

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4 INTERNATIONAL ACTIVITIES

Surveys of international projects, field and laboratory experiments, and collaborations were undertaken to gain familiarity with and leverage research efforts on coupled processes associated with deep disposal over the past two decades in a wide range of geologic media. Although a large number of small-scale or laboratory-based tests were associated with the larger scale *in-situ* field tests, the information in this section emphasizes the large-scale *in-situ* field tests. This review focuses on thermal tests relevant to coupled processes. Isothermal or thermal field tests that focus on a single process, such as producing a thermally perturbed environment at waste package surfaces for testing corrosion processes, are not considered.

The following two subsections cover prominent laboratory and field tests that have a thermal perturbation component. Section 4.1 covers the tests separated by host geologic media: argillite, crystalline, and salt. Overlap necessarily occurs between the buffer and geologic media (i.e., argillite or crystalline rock) tests. Therefore, tests in the buffer are not called out separately, but rather are included in the subsections on argillite and crystalline host media to avoid redundancy. Section 4.2 summarizes activities of the Development of Coupled Models and Their Validation Against Experiments (DECOVALEX) project, some of which are mentioned in Section 4.1.

4.1 Significant Projects/Field Tests

There are two reasons to focus a summary of international activity for coupled processes on large-scale field experiments. First, field experiments typically are a culmination of detailed small tests (i.e., they utilize numerous small-scale or laboratory experiments that focus on separate aspects of processes or conditions). Information on large-scale demonstration field tests often includes the supporting laboratory and small-scale tests. Thus, an information trail is created. The notion of test culmination aligns with the maturity of testing done at underground research facilities that have operated for two decades or more. Second, large-scale field tests address the issue of upscaling of parameters and conditions for a more relevant treatment of space and time scales than the laboratory tests. The large-scale mockup or demonstration experiments at underground research facilities are, by design, representative of situations that are close to those of the expected repository conditions: at least closer than smaller, tightly controlled laboratory tests. This is an important aspect of confidence building for modeling coupled processes.

Information for argillite, crystalline, and salt underground research facilities in this section was gathered from (i) site-specific websites, (ii) literature from peer-reviewed journals and conference proceedings, and (iii) documents completed by waste disposal programs from different countries and regional entities (i.e., European Commission) and international organizations such as the International Atomic Energy Agency (IAEA) and Nuclear Energy Agency (NEA). The information from some site-specific websites for underground research facilities or laboratories necessarily had to be extensively supplemented with other literature because the websites were clearly created to disseminate information to the public. Journal articles and summaries from IAEA, NEA, and European Commission projects provided the detailed technical information. Other site-specific websites for underground research facilities contained abundant technical information or direct links to program documents. For example, the HADES, Mont Terri, and Grimsel websites provide abundant useful information on activities and research documents. IAEA and NEA websites include search tools and links for their documents. The CORDIS website (http://cordis.europa.eu/home_en.html) is an electronic library of project reports and conference proceedings funded by the European Commission.

The following summaries of thermal tests in underground facilities or laboratories are separated by host rock type: argillites (Table 4-1), crystalline rocks (Table 4-2), and salt (Table 4-3). Tests with buffer material are added to the tables for argillite and crystalline rock, as appropriate, though a short discussion is provided in a separate subsection for buffer.

Argillites

Four countries have underground facilities in plastic or indurated argillite formations. The facility or laboratory name, website, and documents with supplemental technical information for each site are

- Belgium: HADES (High-Activity Disposal Experiment Site), Mol
  - http://www.euridice.be/eng/00home.shtm
  - Chen, et al., (2011); Li (2010); Li, et al., (2007); Laine and Karttunen (2010); Bernier and Demarche (2006); Jorda, et al., (1990); Zhang, et al., (2008)

- France: Bure, Meuse/Haute-Marne Departments
  - http://www.andra.fr/andra-meusehautemarne (In French only)
  - http://www.andra.fr/download/andra-international-en/document/editions/182.pdf

- France: Tournemire, Ardeche Department
  - http://www.irsn.fr/FR/base_de_connaissances/Installations_nucleaires/dechets-radioactifs/station_experimentale_tournemire/Pages/sommaire.aspx (French)

- Japan: Honorobe Underground Research Center, Gifu
  - http://www.jaea.go.jp/english/04/horonobe/report.html
  - Kunimaru, et al. (2010)
  - Facility under construction; may be completed in 2010

- Switzerland: Mont Terri
  - http://www.mont-terri.ch/ids/default.asp?TopicID=72

As with Sections 2 and 3 of this report, the term argillite is used broadly here to include plastic clay layers, true argillites, and fissile shale rocks. The underground facility at the Belgian site is in plastic clay, whereas the other sites are in a more indurated rock, such as argillite or shale. Table 4-1 lists thermal tests at each underground facility. The underground facility in Japan (Honorobe) in argillite rock has planned thermal tests, but the underground facility is still under construction.

Table 4-1. Argillite Hosted Underground Facilities and Significant Thermal Field Tests

URL* Name and Location	Lead Country and Agency	Tests
HADES (High-Activity Disposal Experiment Site) Mol-Dessel	Belgium EURIDICE	BACCHUS (Backfilling Control and Heater Experiment for Underground Storage): • *In-situ* backfill/heater experiment from 1988–1989 • Natural Ca-smectite mixed with sand and graphite was used as buffer • Maximum temperature ~95 °C [203 °F] • Measured swelling and water pressure, humidity, and temperature OPHELIE (On surface Preliminary Heating simulation Experimenting Later Instruments and Equipment): • Early full-scale mockup to test equipment, buffer material, and hydration • Dimensions: 5-m [16-ft] length and more than 2-m [6.4-ft] diameter; heating to more than 100 °C [212 °F] • Decommissioned in October 2002 • As with BACCHUS test, one conclusion is that temperatures above boiling should be avoided because of complex phenomena CACTUS (Characterization of Clay under Thermal loading for Underground Storage): • Large borehole, test completed 1994 • Focus on THM processes in Boom Clay • Temperature: 140 °C [284 °F] at the source and 20 °C [68 °F] at 1.5 m [4.9 ft] from heater • Field and laboratory tests under heating indicate no mineralogy change after 5 years, but changes in pore water chemistry for a short period of oxidation and (increase sulphates and pH drop) then chemistry reestablished (to similar to natural) CEREBUS: • Heater and irradiation test from 1986–1998 in Boom Clay focused on effect of emplacing an HLW-canister on the near-field environment • Experiment used a 0.45 × 106 GBq Co-60 source combined with an electrical heating system vertically emplaced in a cased hole in the floor of a drift • Maximum test temperature was 80 °C [176 °F] CORALUS (CORrosion of alpha-Active gLass in Underground Storage conditions): • Duration: 1997–2014 • Project involves an integrated *in-situ* corrosion test including backfill materials exerting a high swelling pressure at controlled temperature {30 and 90°C [86 and 194 °F]} ATLAS (Admissible Thermal Loading for Argillaceous Storage): • Series of tests to evaluate THM effects in the Boom Clay • Duration: started in the early 1990s, and still going as of 2010 • Atlas II temperatures of 70 °C [158 °F]

Table 4-1. Argillite Hosted Underground Facilities and Significant Thermal Field Tests (continued)		
URL* Name and Location	**Lead Country and Agency**	**Tests**
		PRACLAY (Preliminary demonstration test for CLAY disposal of highly radioactive waste): • Heater and seal test (2011–2021) involves gradual heating of a 30-m [96-ft] tunnel to a maximum temperature of 80 °C [176 °F] • Evaluates THMC behavior of Boom Clay and MX-80 bentonite buffer
Bure, Meuse/Haute Marne	France ANDRA	Creep Tests: • In laboratory at temperature up to 120 °C [248 °F] • Literature and experiments indicate no mineral alteration in 20 to 80 °C [68 to 176 °F] range; clay was stable below 200 °C [392 °F] (dehydration and reversible changes) TER Test: • THM processes in horizontal borehole (similar to HE-D test at HADES) • Temperature ~ 50 °C [122 °F] • Test integrates performance of clay core, concrete plug, and buffer material (2007–2009)
Tournemire, Ardeche Dept.	France IRSN	• Experiments are designed include evaluation of damage caused by the excavation of a gallery and / or drying of the rock due to natural ventilation (HM processes). • Additional details not available as most of the information is in French
Mont Terri Rock Laboratory	Switzerland SwissTopo	HE-B, C—Heater Tests: • Focuses on THM processes in host rock/buffer • Vertical borehole in floor {0.3-m [1-ft] diameter} • Maximum temperature of 100 °C [212 °F] • Test volume hydrated with synthetic water for approximately 3 years before heating started HE-D THM Behavior of Host Rock: • Horizontal borehole {0.3-m [1-ft] diameter} • 2 heaters in direct contact with shaly Opalinus Clay host rock • Peak temperatures ~53 and 41 °C [127 and 106 °F] HE-e Experiment: • Focuses on THM processes in microdrift with heaters surrounded by buffer • Two sections of drift to contain different buffer material • Maximum planned temperature is 135 °C [275 °F] • Proposed DECOVALEX-2015 task FE Test: • Planned full-scale emplacement demonstration test with bentonite, shotcrete, steel ribs, anchors • Duration: 10–15 years' heating • Evaluating HM/THM processes with focus on resaturation and stress field including effect of heterogeneity • Extension of drift used in mine; constructed 2010/2011

Table 4-1. Argillite Hosted Underground Facilities and Significant Thermal Field Tests (continued)

URL* Name and Location	Lead Country and Agency	Tests
		TH-A Test: • Microscale-based THMC Twin Hole Disposal Configuration Test: • Initiated in 2009 • Objective is to represent disposal sequence (i.e., one borehole is filled and heated while the second one is kept open for a specified period before it is filled and heated) • Evaluate two different buffer materials for their suitability as a sealing material • THM parameters monitored in emplacement and observation boreholes Application of geophysical tools for EDZ characterization

*URL: Underground Research Laboratory

Table 4-2. Crystalline Rock Hosted Underground Facilities and Significant Thermal Field Tests

URL* Name and Location	Country and Agency	Test
Atomic Energy of Canada Limited (AECL) URL, Pinawa	Canada AECL	Heater test in granite demonstrated limited expansion of EDZ† due to thermal loading.
ONKALO, Olikuoto	Finland Posiva Oy	PORE: • Focuses on TM processes • Monitoring displacement in heated, vertical borehole pair • Temperature: Currently at 50 °C [122 °F]
Kamaishi	Japan	THM Buffer Test: • Excavated pit in drift floor with single analog waste package (heater) vertically emplaced and surrounded by bentonite buffer • Heated 250 days to 100 °C [212 °F], cooling phase for 180 days • Data used in DECOVALEX-III task
KURT	Korea KAERI	*In-situ* Buffer THM Test: • Investigate (i) the THM behavior in a bentonite buffer; (ii) the applicability of a computer code for a THM analysis, and (iii) the engineering feasibility of installing bentonite blocks into a deposition hole (i.e., large vertical borehole in floor of drift) • Planned maximum temperature not known, though a single borehole heater pretest anticipated to exceed 100 °C [212 °F]

Table 4-2. Crystalline Rock Hosted Underground Facilities and Significant Thermal Field Tests (continued)		
URL* Name and Location	**Country and Agency**	**Test**
Stripa Mine Project	Sweden	Effect of Pressure and Temperature on Rock Permeability: • Evaluate THM processes • Tests of the local effects of pressure and temperature gradients on rock permeability Thermal Stress: • Evaluate TM processes • Effects of local heating on changes in the rock stresses and fracture conditions that occur in a rock formation Full-Scale Heater Experiments: • Evaluate TM processes • Investigation of the short-term temperature effects in granite by using a full-size canister that can simulate the energy output of radioactive waste Time-Scaled Heater Experiment: • Evaluate TM processes • Investigation of a long-term thermal loading effect on a rock mass at significant depths
Äspö Hard Rock Laboratory	Sweden Svensk Kärnbränslehantering AB (SKB)	ASPE: • Focus on TM processes • Monitoring geomechanical displacement in paired vertical borehole Prototype Repository Test: • Duration: 2001 to present; emplacement in 2001 and 2003, and excavation 2011 • Complete mockup including 6 vertical boreholes and backfill of tunnels • Reopened due to heater failures • Some chemical data collected in buffer, backfill, and host rock besides HM measurements LOT Experiment (Long-Term Test of Buffer Material): • Seven vertical boreholes • Temperature: Heaters and buffer at 90 °C and 120–150 °C [194 °F and 248–302 °F] • Measure hydro parameters, temperature, potassium concentration, pH, accessory minerals • Posttest excavation for mineralogical analysis Alternate Buffer Material: • Compare different buffer materials emplaced in vertical borehole • Temperature: At heater 130 °C [266 °F] • Compare mineral stability and physical properties • Study buffer interaction with metallic iron and bentonite

Table 4-2. Crystalline Rock Hosted Underground Facilities and Significant Thermal Field Tests (continued)		
URL* Name and Location	**Country and Agency**	**Test**
		<u>Temperature Buffer Test</u>: • Two adjacent bentonite buffer tests in large vertical boreholes • THM for upper package and THMC for lower package • Temperature: Heated to above 100 °C [212 °F] during saturation process • Dismantling in 2009 and 2010 for additional data
Grimsel Test Site	Switzerland Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA)	<u>FEBEX (Full-scale Engineered Barriers Experiment)</u>: • Consists of an *in-situ* full-scale engineered barrier system (EBS) test performed under natural conditions • Evaluating THMC processes in the bentonite buffer focusing on the role of thermal convection, the onset of corrosion/gas production, gas transport capacity of the near-field (saturation history) and the geochemical evolution of the near field (e.g., iron/bentonite interactions) • Maximum temperature 100 °C [212 °F] at bentonite–canister interface • Duration: 1994 to present. • FEBEXe, 2003–2013; extension of FEBEX full-scale engineered barriers experiment
DUSEL Homestake Mine, South Dakota	USA University of California, Berkeley (THMC component)	<u>Coupled THMC-Biological Experimental Facility:</u> • Large-scale THMCB (THMC and biological) test currently at initial stage of design and instrumentation • The fractured rock volume that will be heated has dimensions of 50 × 40 × 40m [164 × 131 × 131 ft] • Heating expected to start 2013 • Planned maximum temperature range 150–300 °C [302–572 °F]
*URL: Underground Research Laboratory †EDZ: Excavated Damaged Zone		

Table 4-3. Rock Salt Hosted Underground Facilities or Salt Laboratory Tests With Significant Thermal Component		
URL* Name and Location	**Country**	**Test Description**
Asse Salt Mine	Germany	Analyses and modeling done under BAMBUS-II Project <u>TDSE (Thermal Simulation of Drift Emplacement)</u>: • Full-scale THM tests in two parallel drifts backfilled with crushed salt • Constant heat source raised temperatures up to 210 °C [410 °F]; after 5 years, temperature dropped to 170 °C [338 °F] • Assessed creep rate, backfill compaction, and stress field • Assessment of water and gas releases from the backfill material revealed significant increases of carbon dioxide, methane, and hydrogen concentrations due to heating <u>DEBORA (Development of Borehole Seals for Radioactive Waste)</u>: • TM damage zone and evolution of sealing with crushed salt • Temperatures up to 140 °C [284 °F] • Evaluated crushed salt compaction in deep borehole; comparison of salt compaction in borehole versus that in the seal (expect temperature difference between the two) • Observations of porosity and permeability changes

Table 4-3. Rock Salt Hosted Underground Facilities or Salt Laboratory Tests With Significant Thermal Component (continued)		
URL* Name and Location	**Country**	**Test Description**
		HAW (High Active Waste): • Borehole emplacement in drift floor • Duration: 5 years • Focused on TM behavior • Maximum temperature of 230 °C [446 °F] (per test plan)
Russian Lab Test	Russia	• Thermal test at a laboratory scale • Evaluate brines and vapor migration near analog waste packages • Temperatures up to 200 °C [392 °F]
WIPP	USA	(D)HLW Mockup: • Designed to study effects of heat on room closure, structural stability, and waste encapsulation, using the exact thermal and structural load of a reference repository design • Three-drift configuration • Based on the number of heaters and wattage, temperatures estimated to be substantially less than those for the DHLW Overtest DHLW Overtest: • Accelerated version of (D)HLW Mockup Test performed by applying fourfold increase in thermal load using the middle drift of the DHLW Mockup Test; focused longer term behavior and creep rate and heat transfer at higher temperatures • Canister–salt interface temperature reached 250 °C [482 °F] • Posttest recovery of canisters retained for corrosion analysis Heated Axisymmetric Pillar Test: • Data collected on a 190-m^3 [6,700-ft^3] pillar heated to 70 °C [158 °F] for 10 years • Objectives included (i) model validation for predicting accelerated creep in pillar and room due to heat (ii) mechanical properties and failure modes of salt and other constituents, and (iii) comparison of actual 3D response to 2D models Crushed Salt Reconsolidation: • Laboratory tests at elevated temperatures and pressures {up to 250 °C [482 °F] and 20 mB [0.3 psi]} performed to complement tests in the 1980s at temperatures below 100 °C [212 °F] • Objective was to support extent, rate, and fundamental understanding of reconsolidation of crushed salt backfill

*URL: Underground Research Laboratory

Most tests for argillite generally focus on uncertainty of (i) damage zone extent, (ii) healing of damage, and (iii) processes at buffer–host rock interface. Maximum temperatures for the field tests were kept below 140 °C [284 °F]. This limit on the maximum temperature is a design constraint probably related to the possibility of clay dehydration (removal of bound water) and increased kinetics rate for mineralogic alteration of the clays.

Two recent or ongoing projects that utilize information and data from several *in-situ* tests at different underground facilities are Thermal Impact on the Damaged Zone Around a Radioactive Waste Disposal in Clay Host Rocks (TIMODAZ) and Long-Term Performance of Engineered Barrier Systems (PEBS). TIMODAZ has been active from 2006 through 2010 (Li, et al., 2007). TIMODAZ encompasses information from literature, laboratory, and field tests. This project compared THM behavior, and in some cases geochemical behavior, in the damage zone of the host rock of Boom Clay, Opalinus Clay, and Callovo-Oxfordian Clay, which are the host formations at the underground facilities of Belgium, Switzerland, and France, respectively. Maximum temperatures of tests used in the TIMODAZ project ranged up to 80 °C [176 °F]. One component of the TIMODAZ project was to predict expected behavior of the PRACLAY test that was to begin at HADES in 2011.

The PEBS project is designed to evaluate sealing and barrier performance at three times in evolution of the engineered barrier system (http://www.pebs-eu.de). The three repository times and corresponding *in-situ* tests are (i) early resaturation as represented by the HE-e model validation test, (ii) the resaturation period (~50 years) as represented by a FEBEX-type mockup test expected to run for 15 years, and (iii) the pressure recovery period (>200 years) as represented by the EB experiment. The HE-e test will start in 2011 and has been proposed as a task for the DECOVALEX-2015 collaborative project.

<u>Buffer</u>

Most European and Asian countries with a disposal program are considering a repository design with buffer material surrounding the waste package, with the exception for salt repository designs, such as those used in the German program. Thus, buffer material is a common component of thermal testing in underground facilities for argillite and crystalline host rocks. Cement either associated with the emplacement area or with seals for the emplacement boreholes is also integrated into repository designs and thermal tests.

Many tests at the underground facilities focus on understanding mechanical, chemical, and hydrological changes in the buffer. Resaturation and swelling behavior of buffer during the thermal period depends on the type of buffer material and the packing density. Engineered buffer material offers homogeneity and cation exchange control. Prominent thermal tests and maximum temperatures are (i) the FEBEX full-scale mockup tests at Grimsel {100 °C [212 °F]}, (ii) a series of tests of different buffer materials and packing techniques at Aspo {90–130 °C [194–266 °F]}, and (iii) the planned HE-e and FE tests at Mont Terri {135 °C [275 °F]}.

Natural bentonite deposits offer insights into buffer evolution over long time periods. A recent survey by Posiva Oy (Laine and Karttunen, 2010) provides an extended discussion of the properties and long-term stability of bentonite. It was suggested that studies of natural bentonite deposits near heat sources would help constrain reaction rates for smectite conversion to illites.

Cement is a part of waste disposal designs for several countries, either as a component of seals, drift support, or waste package system (e.g., the Belgian Super Waste Package). Accordingly, cementitious material is also a component of several field tests (e.g., FEBEX).

Two projects at underground research facilities and one analog site that address bentonite–cement interaction follow.

- Long-term Cement Study (LCS) (Grimsel 2006–2013): This project includes laboratory and field experiments to increase the understanding of high-pH cement interaction effects in the repository near field and the geosphere.

- Mont Terri Cement–Clay Interaction (CI) Project: This long-term cement interaction experiment was conducted in two boreholes in the Opalinus Clay.

- Maqarin Analog Site (Jordan): Fractures were sealed by calcite due passage of high pH fluids. Cement was deposited due to high temperature fluids. The THC modeling focused on redistribution of cement by subsequent low temperature fluids (e.g., Steefel and Lichtner,1998; Alexander, et al., 2005).

Crystalline

Sweden, Finland, Switzerland, Japan, and Korea have developed or are developing underground facilities in crystalline rocks. The facility or laboratory name, website, and documents with supplemental technical information for each site are

- Canada: Atomic Energy of Canada Limited (AECL) Underground Research Facility, Pinawa
  — IAEA (2001)

- Finland: ONKALO, Olkiluoto
  — http://www.posiva.fi/en/research_development/onkalo

- Japan: Kamaishi Mine
  — Chijimatsu, et al. (2001)

- Japan: Mizunami Underground Research Laboratory, Tono Geoscience Center
  — Sugihara (2009)
  — Currently under construction. Thermal test is planned.

- Korea: KURT
  — KAERI
  — http://ehome.kaeri.re.kr/snsd/eng/institution/institution3.htm
  — Cho, et al. (2008); Kwon, et al. (2011)

- Sweden: Stripa Mine Project, 1976 to 1992
  — Hardin (1992)

- Sweden: Aspo Hard Rock Laboratory
  — SKB (2010)
  — http://www.skb.se/Templates/Standard____25506.aspx

- Switzerland: Grimsel
  - http://www.grimsel.com

- USA: DUSEL (Deep Underground Science and Engineering Laboratory), Homestake Mine, South Dakota
  - http://www.dusel.org/html/science.html

For Finland, France, and Sweden, heater tests in crystalline rocks are listed in Table 4-2. The underground facility in Japan (Tono, Mizunami, and Gifu) has planned thermal tests in crystalline rocks, but the underground facility is still under construction so it is not listed in Table 4-2. The underground facility in Korea [Korean Atomic Energy Research Institute (KAERI) Underground Research Tunnel (KURT)] has been constructed, and its heater test, which includes a buffer, is being instrumented; however, it is still listed in Table 4-2.

Prominent mockup (full-scale, emplacement design) tests in crystalline rocks include the FEBEX series at Grimsel and the PROTOTYPE Repository Test at Aspo (Gens, et al., 2004). Both include bentonite buffer of various types. Active collaborative projects include the European Commission-funded NF-Pro project and the SKB-sponsored Engineered Barrier System (EBS) Task Force. The NF-Pro project tasks focus on near-field processes by analyzing several tests covering the evolution of a repository (i.e., tests representing the operational period, early post-closure period, and long-term behavior) (European Commission, 2008). The EBS Task Force   focuses on THM modeling during water transfer between buffer, backfill, and near-field rock and on gas transfer in saturated buffer (Steefel, et al., 2010). The EBS Task Force is composed of organizations from eight countries. It started in 2004 and meets twice a year to discuss progress and possible new areas of research.

Salt

The United States and Germany have underground facilities in salt and are the primary countries that have such programs. Spain has considered salt as a host material for disposal, but has no underground facility. The countries, site names, and information sources for salt are

- Germany: Asse II Mine
  - Bechtold, et al. (2003); Rochfuchs, et al. (1998, 2004)

- USA: Waste Isolation Pilot Plant (WIPP), New Mexico
  - www.wipp.energy.gov/science/repository/RepositoryNew.html
  - Matthews and Eriksson (2003); Clayton, et al. (2010)

- Russian Laboratory Test
  - Schneider (2010)

The WIPP site in the United States and the Asse-II Mine in Germany included both testing programs and storage of radioactive waste, albeit not high-level waste. Thermal tests associated with each of these sites are listed in Table 4-3. Testing focuses on (i) stability of the opening, including the disturbed rock zone, and creep rate for cavern closure at ambient and elevated temperatures and (ii) performance of seals for keeping far-field flow disconnected from the near field (Matthews and Eriksson, 2003). Maximum temperatures reached in the thermal tests listed in Table 4-3 cover the range from above ambient to 240 °C [464 °F].

Important projects in salt host rock were BAMBUS-II and THERESA. The BAMBUS-II project analyzed and simulated laboratory data and all three field-scale tests at the Asse II mine (Bechthold et al 2003; Stuhrenberg and Heusermann, 2004). The European Commission-funded THERESA collaborative project (2005–2009) focused on comparing alternative models using test data from the Asse II mine. Documentation from THERESA is complete, but has not yet been released for publication.

4.2 International Collaboration: Development of Coupled Models and Their Validation Against Experiments

In a survey of international collaborative projects, active projects DECOVALEX, PEBS, and EBS Task Force were identified. Other collaborative projects, such as the Clay Club, Natural Analogue Working Group, and Thermodynamic Database Project, are peripherally related to modeling of THMC coupled processes, but are not mentioned further in this report. Numerous completed projects were identified in the survey, each of which provides informative documentation of past work. However, active projects provide an opportunity for NRC to leverage international experience and gain peer relations with staff from organizations from other countries. The DECOVALEX collaboration (i) provides a broad spectrum of involvement from the international community, (ii) involves task topics that focus on THMC coupled processes, and (iii) is the most cost-efficient active collaborative group to join.

The DECOVALEX collaborative project started in 1992 and is currently in the fifth phase. Each phase lasts 3–4 years and has three to six separate tasks. The tasks for the five DECOVALEX phases are summarized in Table 4-4 along with associated documentation. NRC participated in Phases I and III. Experimental data from a hydrological test on a fracture under stress that was performed at CNWRA were used in DECOVALEX Phase I (Table 4-4, Task 2). For each phase, participants formulate tasks that are of interest to the individual countries, yet would also be of interest to other organizations. The goals and methodology of DECOVALEX are directed toward coupled THMC processes in host rock and buffer for deep geologic repositories. The objectives are (i) to validate approaches using measured data from field and lab experiments and (ii) to compare alternative methods and representations used among different participants.

DECOVALEX tasks may be either (i) field or laboratory experiments or (ii) benchmark tests; the former incorporates measured and observed data from tests and the latter is the formulation of a hypothetical scenario. Benchmark tests are more conducive to addressing questions pertaining to the importance of inputs or processes to performance or safety assessments.

Early phases focused on HM, TM, and THM modeling of laboratory and field tests, including development of THM codes. Rock mechanics appeared to be a prominent focus of the group in early phases. One of the tasks in DECOVALEX-II phase and three tasks in DECOVALEX-III phase addressed performance aspects of THM, MH, and THMC processes. Later DECOVALEX phases continued the THM emphasis, but also tried to incorporate more tasks with geochemical components—something that continues to be of interest based on preliminary discussions for tasks in phase 6 (DECOVALEX-2015). However, quality THC or THMC data from experiments are sparse, especially at temperatures between 100 and 200 °C [212 and 392 °F].

DECOVALEX-2015 will start in 2012. Interested potential participants are currently discussing tasks for this new phase. NRC considerations for selecting or modifying a task include (i) the task(s) should cover a wide range of applicability in different geologic media and repository

Table 4-4. Development of Coupled Models and Their Validation Against Experiments Tasks and Documentation for Each of Five Phases

Phase	Tasks	Documentation, Books, or Journal Volumes
DECOVALEX I 1992–1995	1. Three BMT* problems: THM† processes in fractured rock with three different fracture patterns 2. Three test cases of mechanical effects on flows in a single rock joint (lab experiments provided by NRC and CNWRA) 3. One test case on an experiment of THM processes in a fractured rock 4. Big-Ben experiment of THM processes in engineered buffer materials 5. One test case on an *in-situ* borehole injection experiment in a fractured rock	Stephanson, O., L. Jing, and Tsang, C.-F. *Coupled THM Processes of Fractured Media: Mathematical and Experimental Studies.* Atlanta, Georgia: Elsevier. 1995. IJRMMS‡, Vol. 32, No. 5, 1995.
DECOVALEX II 1995–2000	1. Shaft excavation on HM at Sellafield, UK 2. *In-situ* THM experiments at Kamaishi Mine, Japan 3. Review of state of the art of constitutive modeling of rock joints 4. Current understanding of THM processes related to performance of nuclear waste repositories	IJRMMS, Vol. 38, No. 1, 2001.
DECOVALEX III 2000–2003	1. FEBEX experiment at Grimsel Mine, Switzerland (heater test in granite with bentonite buffer) 2. Yucca Mountain Drift-Scale Heater Test 3. BMT 1: Effect of THM processes on near-field performance 4. BMT 2 and 3: Effects of homogenization and upscaling of MH properties and glaciation on far-field performance and safety assessments 5. THMC† processes in safety assessment	Stephansson, O., J.A. Hudson, and L. Jing. *Coupled THMC Processes in Geo-Systems–Fundamentals, Modelling, Experiments and Applications.* Atlanta, Georgia: Elsevier. 2004. IJRMMS, Vol. 42, Nos. 5–6. 2006.
DECOVALEX-THMC 2004–2007	1. Influence of near-field THM processes on performance assessment 2. HMC† studies of the excavation disturbed zone 3. Excavation damaged zone in the argillaceous Tournemire site, France 4. Permanent permeability/porosity changes due to THMC processes 5. THM processes from long-term climate change: glaciations case study assessment	Journal of Environmental Geology, Vol. 57, No. 6, pp. 1,217–1,389. 2009.
DECOVALEX-2011 2008–2011	1. THMC processes in bentonite buffer in argillaceous rock, Mont Terri, Switzerland 2. Pillar stability & fracturing in a granite rock under heating, Äspö, Sweden 3. Bedrichov Tunnel, Czech Republic a. 2D benchmark test of coupled stress-flow-particle transport b. A test case on 3D flow modeling of Bedrichov water conducting tunnel in fractured granite in Czech Republic	Documentation unavailable

*BMT: Benchmark Test
†THM/HMC/THMC: Thermal-Hydrological-Mechanical-Chemical
‡ IJRMMS: International Journal of Rock Mechanics & Mining Science

designs (i.e., the developed tools and expertise are widely applicable); (ii) the task(s) should include a performance insight portion; and (iii) the task(s) should include a geochemical component. Although other potential tasks were discussed in the October 2010 and April 2011 DECOVALEX workshops, the three tasks that may fit these considerations include

- FEBEX (or other old task) at Grimsel
  - THMC processes in buffer and buffer/granitic host rock interface; 100 °C [212 °F]
  - At the NRC/CNWRA THMC Workshop March 31, 2011, staff discussed the potential use of this experimental data set to help guide development of THC and THM tools over the next two years in preparation for DECOVALEX-2015

- HE-e at Mont Terri
  - THM/C buffer and buffer/argillite host rock interface; 135 °C [275 °F]
  - At the NRC/CNWRA THMC Workshop March 31, 2011, staff discussed the information needs for expanding the proposed task to include
    - Identify the gap in thermodynamic data for MX-80 or FEBEX-type bentonite at an elevated temperature in the range of 135 to 200 °C [275 to 392 °F]
    - Identify performance insights that could be addressed using the developed THC and THM tools and the HE-e test design, but at higher temperatures

- SEALEX test at Tournemire
  - HM only; buffer and buffer/argillite host rock interface
  - Focus on swelling, saturation, and possible flow in bentonite seals at emplacement boreholes; seals includes cement component for structural support
  - Not a thermal test

Discussion during and after the NRC/CNWRA Workshop of March 31, 2011, is intended to support a potential NRC modification of a proposed task in the summer of 2011 and the selection of a task at the next DECOVALEX workshop in November 2011.

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5 SUMMARY

To become better prepared for a variety of possible future directions of the nation's waste disposal program, staff are reviewing available literature on a range of geological media and conceptual repository designs. This report summarizes available information on coupled processes associated with deep disposal of waste in different geologic media. Much of the information in this report was presented and discussed in an NRC/CNWRA THMC workshop held March 31, 2011.

Geologic media, broadly categorized into crystalline rock, argillite rock, and salt are being considered as host rocks for radioactive waste disposal. The functions of the host medium and buffer/backfill materials include (i) isolating wastes from the near-surface environment; (ii) maintaining geochemical, hydrogeological, and geomechanical environments favorable to the preservation and performance of the EBS; and (iii) acting as a natural barrier restricting water access to the wastes and the migration of mobilized radionuclides. THMC coupled processes can affect the ability of the host medium and buffer/backfill materials to isolate the waste and mitigate the migration of radionuclides. Understanding these couplings of processes is essential for reliably assessing repository performance and evaluating the safety case.

Argillaceous clay-rich rocks are considered as potential repository host rocks because of their favorable hydrologic (low permeability), chemical (low diffusion coefficient), and mechanical (capability to self-seal fractures in the damaged zone) properties. The drying and resaturation processes, controlled by TH coupling, extend for long durations because of low permeability and porosity of argillites. THC/HC coupled processes affect (i) transformation of smectite to illite that could lead to an embrittlement and a partial or total loss of swelling capacity; (ii) dissolution/precipitation reactions and clay mineral alteration that could change the hydraulic conductivity of the argillite; (iii) changes in the pore water chemistry that could affect radionuclide solubility and sorption, waste package corrosion, and waste form degradation; (iv) modification of the ion-exchange, hydration, and swelling behavior of the clay minerals; and (v) alteration of clay colloid stability. Rock fracturing due to excavation, thermal loading, or drying shrinkage could affect water flow and pore pressure dissipation because of the enhanced hydraulic conductivity. Furthermore, a change in pore water pressure due to drainage, imbibition, or thermal expansion could affect fracturing or fracture healing. Therefore, estimating damage-zone evolution in argillaceous rock entails coupled THM modeling.
Based on current staff understanding, the dominant THMC processes for argillites include the (i) TH coupling that refers to the influence of thermal load on the rate of saturation and desaturation processes; (ii) TC coupling that refers to the temperature-dependent chemical characteristics such as solubility and sorption coefficients and clay mineral and colloid stability; (iii) TM coupling that influences the rate of swelling (thermal expansion); and (iv) THM/HM coupling that refers to the influence of saturation on development of pore pressures, that in turn, controls the swelling process.

Bentonite or a bentonite–sand mixture is proposed as a buffer and backfill material in a number of countries. The hydrological (low hydraulic conductivity), geochemical (very low diffusion, high sorption, good colloid and microbial filtration capability), and mechanical (high swelling potential enables self-sealing of openings) properties of bentonite make it a favorable buffer/backfill material between the waste packages and host formation. Similar to the argillites, drying and resaturation rates are controlled by TH coupling and buffer design. These processes are very slow because of low buffer permeability and presence of a thermal gradient. The main TC effect on bentonite may be heat-induced transformation of montmorillonite to either beidellite or illite, which could lead to embrittlement, a partial or total loss of swelling capacity, and an increase in hydraulic conductivity of the clay material. Higher temperatures also could (i) enhance dissolution/precipitation reactions that could alter the hydraulic conductivity and possibly create preferential flow paths in the bentonite buffer/backfill; (ii) change pore water chemistry that could affect radionuclide solubility and sorption, waste package corrosion, and waste form degradation; (iii) modify the ion-exchange, hydration, and swelling behavior of the clay minerals; and (iv) alter clay colloid stability. Cracking in the buffer could occur because of (i) desiccation or crack healing due to swelling and (ii) frictional resistance at buffer vertical walls due to loss of vertical confinement. Cracks in the buffer subjected to high water-flow velocities could result in internal erosion of buffer. Therefore, estimating buffer damage due to cracking and internal erosion entails coupled THM modeling. Based on current staff understanding, the dominant THMC processes for buffer/backfill include (i) the TH processes that affect the spatial and temporal distribution of the saturation during the drying and rewetting of the buffer during the initial postclosure period; (ii) the degree of swelling is controlled by the HM coupling with a strong impact of the thermal pulse; (iii) the THC/TC coupling that determines the chemical composition of the buffer, which impacts the retardation capabilities of the buffer (sorption, solubility, colloid properties); and (iv) the TMC coupling that could cause changes in mechanical properties for above-boiling conditions.

Cementitious materials are major components of engineered barriers or structures in most low-level waste, intermediate-level waste, and transuranic waste geologic disposal repositories and in some high-level waste repository concepts. These materials are used in repository vaults, floors, tunnel linings and plugs, waste conditioning matrices, and backfill. Because of the alkaline pH of cement pore waters, interaction with crystalline and argillite host rocks and with clay buffer/backfill is an important geochemical process that needs to be considered in performance assessments. The alkaline pH of cement pore waters could alter the host rock mineralogy and buffer/backfill properties. THC/HC couplings include the dissolution and precipitation processes that result in porosity/permeability changes that alter groundwater/gas flow pathways in the host rock and buffer/backfill. Interaction of groundwater with cementitious materials also could change the water chemistry and affect radionuclide solubility and sorption.

Hydrological (low permeability in unfractured rocks), mechanical (high strength), and geochemical (high sorption and low dissolution) characteristics of crystalline rocks are considered beneficial to repository performance. The flow regime in crystalline rocks is governed by the extent of fracture connectivity and presence of structural features such as faults. THC/HC coupled processes affect (i) several geochemical processes, including radionuclide solubility and sorption and colloid stability and (ii) near-field water chemistry, which would affect waste container corrosion and waste form degradation. Mineral dissolution/precipitation occurring in the near field may change the hydraulic conductivity of the host rock, whereas water chemistry may change due to flow of groundwater with different composition. Porosity and permeability increase in the damaged zone is attributed to stress change due to excavation or thermal loading and could directly affect water pressure and flow. However, the hydrological processes are not likely to have any appreciable effects on rock deformation. Therefore, damage-zone evolution in crystalline rock could be estimated using TM modeling alone. TM modeling need not be coupled with hydrological modeling, if the effects of water pressure changes on deformation and the effects of fracturing on porosity and permeability are accounted for in the TM and hydrological models. Based on current staff understanding, the dominant THMC processes for crystalline formations include (i) TMH coupling that influences the thermal deformations which, in turn, could lead to changes in permeability and porosity; (ii) TH coupling that influences the thermal conduction processes; and (iii) TC coupling that influences the solubility and sorption properties of the host rock.

Salt is considered for a host media because of its extremely low permeability, leading to practically very low flow conditions; this characteristic implies there will be less potential for radionuclide transport. Temperature gradients could result in thermally induced brine flow or two-phase flow. Condensation on cooler waste containers in the chambers could contribute to brine formation, corrosion, and gas generation. Brines that form in a salt repository likely will be corrosive to waste containers, and higher temperatures would increase the corrosion rate. Higher temperature in the near field also could increase the degradation rate of the waste form and other engineered materials (e.g., seals), increase radionuclide solubilities, and decrease radionuclide sorption. On the other hand, mineral dissolution and precipitation could alter the hydrological properties of the salt host rock and flow of groundwater with different composition could change the near-field water chemistry. In addition, changes in the mineralogical composition of the salt host rock could significantly alter its mechanical properties. Deformations need to be evaluated to estimate rock damage or healing that may affect the evolution of fluid flow paths and the environment and loading of waste containers. Mechanical modeling to evaluate deformations need not be coupled with hydrological modeling, but the effects of water pressure in nonsalt layers or zones need to be evaluated. The effects of geochemical healing on mechanical behavior could be important, but include considerable uncertainties. Based on current staff understanding, the dominant THMC processes for salt formations include (i) THM coupling that determines the creep rate that, in turn, causes a change in porosity and permeability; (ii) TC coupling that determines the temperature-dependent solubility and sorption properties of the formation; and (iii) TH coupling that determines the temperature-dependent fluid density and viscosity properties.

Based on information summarized in the previous paragraphs, staff evaluated the capabilities and suitability of selected numerical models that could be used to simulate THMC processes in geologic media and buffer/backfill materials. For argillites, THMC or HM couplings are expected to be important in the near field and THMC coupling would be crucial in the buffer zone. Therefore, staff recommend evaluating TOUGHREACT-FLAC3D, RockFlow/RockMech, ABAQUS, COMSOL, and STOMP for argillaceous host rocks. For crystalline formations, THM or HM coupling is expected to dominate the near-field environment. Therefore, staff also recommend evaluating CONNECTFLOW, COMSOL, ABAQUS, UDEC/3DEC, and TOUGH-FLAC further for crystalline host rocks. For salt formation, THM or HM coupling would be crucial; therefore, ABAQUS, TOUGH-FLAC, or SNL Sierra Mechanics would be suitable numerical codes for such simulations. Staff also evaluated the potential for in-house code development. As an alternative to using existing codes, *xFlo* (an in-house TH code) can potentially be improved by adding geomechanical or geochemical modules for THM and THC simulations.

Surveys of international projects, field and laboratory experiments, and collaborations were undertaken to gain familiarity with and leverage research on coupled processes associated with deep disposal over the past few decades in a wide range of geologic media. Staff compiled information related to prominent laboratory and field tests that have a thermal perturbation component for argillite, buffer, crystalline, and salt as host rock.

A survey of international projects supported NRC joining the Development of Coupled Models and Their Validation Against Experiments (DECOVALEX) group. The goal of the DECOVALEX project is to increase understanding of the THMC process and validate models by simulating large laboratory or field experiments. DECOVALEX-2015 will start in 2012. Interested potential participants are currently discussing tasks for this new phase. NRC considerations for selecting a task for the next stage of DECOVALEX include (i) covering a wide range of applicability given that the geologic media is not known for the U.S. program and (ii) considering or incorporating analyses addressing importance to repository performance. Some of the tasks currently being proposed for DECOVALEX-2015 are being evaluated with respect to NRC considerations.