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- Hydrologic issues related to radioactive waste repositories reviewed
- Progress in flow and solute transport in complex geologic media summarized
- Geologic media considered include fractured rock, unsaturated zone, and clays

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Hydrologic issues associated with nuclear waste repositories

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Abstract Significant progress in hydrology, especially in subsurface flow and solute transport, has been made over the last 35 years because of sustained interest in underground nuclear waste repositories. The present paper provides an overview of the key hydrologic issues involved, and to highlight advances in their understanding and treatment because of these efforts. The focus is not on the development of radioactive waste repositories and their safety assessment, but instead on the advances in hydrologic science that have emerged from such studies. Work and results associated with three rock types, which are being considered to host the repositories, are reviewed, with a different emphasis for each rock type. The first rock type is fractured crystalline rock, for which the discussion will be mainly on flow and transport in saturated fractured rock. The second rock type is unsaturated tuff, for which the emphasis will be on flow from the shallow subsurface through the unsaturated zone to the repository. The third rock type is clay-rich formations, whose permeability is very low in an undisturbed state. In this case, the emphasis will be on hydrologic issues that arise from mechanical and thermal disturbances; i.e., on the relevant coupled thermo-hydro-mechanical processes. The extensive research results, especially those from multiyear large-scale underground research laboratory investigations, represent a rich body of information and data that can form the basis for further development in the related areas of hydrologic research.

1. General Introduction

Significant progress in hydrology, especially in subsurface flow and solute transport, has been made over the last 35 years because of sustained interest in the performance assessment of proposed underground nuclear waste repositories. The present paper attempts to provide an overview of the key hydrologic issues involved and to highlight the advances in their understanding and treatment because of these efforts. This paper is not focused on the development of high-level nuclear waste repositories and their safety assessment; it focuses instead on the advances in hydrologic science which have emerged from such studies. These advances may find applications in other hydrology-related problems of current importance at the national and international levels, such as environmental contamination remediation, carbon dioxide geosequestration, and natural gas production through fracking.

In the next section, we present, in a general way, the context for the hydrologic framework related to performance and safety assessment of underground nuclear waste repositories that are proposed to be constructed in three particular rock formations—crystalline rock, unsaturated tuffs, and clays. Then, we discuss some particularly challenging factors concerning the research common to these three formations. This discussion will be followed by three sections devoted to each of these three rock types, respectively, to present a review of hydrologic research in these areas.

1.1. Context

The need for management and disposal of high-level nuclear waste was recognized right from the time when U.S. Congress passed the Atomic Energy Act of 1954, which for the first time made the development of commercial nuclear power possible. In a seminal report by the U.S. National Academy of Sciences [Hess *et al.*, 1957], wide-ranging issues related to geological repository for nuclear waste were discussed, many of which are still of relevance today. The American Physical Society convened a special panel to review various options for disposal of nuclear waste, which were summarized in a 176 page paper in the *Review of Modern Physics* [Hebel *et al.*, 1978]. In all these and subsequent discussions, waste repositories built several hundred

meters underground were found to be a promising possibility. Among other reasons, the viability of geological disposal is based on the view that the long-lasting radioactivity of these wastes can best be isolated by putting them into an environment which is stable over geological time scales. The optimal choice of land-based deep-underground repositories has been confirmed in a number of more recent high-level committee reports [e.g., *USDOE Blue Ribbon Committee*, 2012].

Over the last three decades, research has been conducted in a number of geological formations to investigate the performance and safety of potential underground repositories for nuclear waste. These include crystalline rock, thick unsaturated zone in tuff, indurated and plastic clays, and dome and bedded salt. The present paper will not dwell on salt formations, because hydrologic issues related to salt are relatively limited. They mainly relate to fluid flow through temporary fractures created by excavation-induced deformation of salt, and these fractures self-seal in a relatively short time due to salt plasticity. Fluid may also migrate through salt in brine inclusions, which have the interesting tendency to migrate up a thermal gradient. Some of these issues are included in a general overview paper by *Tsang et al.* [2005]. The present paper will, however, address hydrologic issues in the other three types of rock formations.

The literature on field, laboratory, and modeling studies related to the performance of a nuclear waste repository in crystalline rock, unsaturated zone in tuff, and clays will be presented in terms of some representative papers in the sections below that are devoted to each of these three rock types. The reason to discuss these three types of formation together in the present paper is that these studies have a common goal, which is an evaluation of the potential of radionuclide leakage from the repositories to the biosphere. A number of international cooperative projects, such as the DECOVLAEX project [*Stephansson et al.*, 1996; *Tsang*, 2009; *Hudson and Jing*, 2013], were conducted to study all these rock types in one forum with very fruitful exchange of ideas and data. For example, within this forum, sophisticated numerical codes such as the TOUGH-FLAC simulator [*Rutqvist*, 2011] were successfully applied to all three cases, adding significant confidence to simulation results.

The safety of a nuclear waste repository is based on a multiple-barrier concept, which includes first a stable waste canister, then an engineered (or man-made) buffer enclosing the canisters, and finally a natural (or geological) barrier to minimize the transport of radionuclides to the biosphere. A good overview of the optimal design of an underground nuclear waste repository and the approach taken to conduct the safety assessment may be found in *SR-Site* [2011] for the particular case of waste repository in crystalline rock. However, the approach is fundamentally the same for the other rock types. *Neretnieks* [1993, 1994] summarized the issues of importance for nuclear waste repositories in crystalline rocks as seen at that time, and the approaches to obtain data and to increase understanding. Most of the issues presented are still valid, but additional needs have been identified since then [*Birkholzer et al.*, 2012].

1.2. Some Aspects of Repository Research in the Three Rock Types

Witherspoon and Bodvarsson [2006] presented the status of waste repository research activities in many countries in the world. Crystalline or granitic rock is the focus of nuclear waste repository development in Sweden, Finland, China, and other countries. The countries that are considering clays, indurated or plastic, as host formations for waste repository include France, Belgium, and Switzerland. The United States Department of Energy spent over two decades to investigate a thick unsaturated zone in tuff in the state of Nevada for possible development of a waste repository. The evaluation report by the staff of the United States Nuclear Regulatory Commission on the safety after permanent closure was published in October 2014 [*USNRC*, 2014].

As mentioned above, this paper focuses not on repository development and its performance assessment, but on hydrologic issues pertaining to the ability of the natural barrier to deter mobilization of radionuclides from the waste canisters and their transport toward the biosphere. Generally, the main way potential leakage of radionuclides may occur is through the leaching of these radionuclides from waste canisters emplaced in the repository into the surrounding water, and then the water with its dissolved contaminants flows through the geologic formations to the biosphere. Hence, hydrology plays a key role in the evaluation of such potential leakage flow paths.

Crystalline rock is a hard rock with faults and a network of fractures embedded in rock matrix with a very low permeability. Therefore, fluid flow mainly occurs through the network of fractures. These fractures may

be present in different sizes, ranging from microfractures of centimeters in length, which may not be connected and thus contribute little to flow permeability, to major fault zones kilometers in extent and many meters in thickness. The matrix and microfractures, while having low permeabilities, could play an important role in solute transport by providing the pore space for solute diffusion and hence transport retardation. At the depth of the repository, generally on the order of 500 m, the rock is saturated with water, and so water is available around the waste canisters in a relatively short period after the repository is filled with waste canisters and then sealed and closed. Thus, the hydrologic issues are mainly related to flow and transport in the saturated fractured rock away from the repository toward the biosphere, and secondly to the incoming flow and transport of solutes to the canister and its waste that may degrade the canister and enhance the dissolution rate of the waste form.

The unsaturated or partially saturated zone in tuff, with a thickness of several hundred meters above the water table at Yucca Mountain, Nevada, USA, was proposed as a possible site for a waste repository. The argument for the unsaturated zone being a good choice for waste disposal was that without the presence of flowing water, the corrosion of the canisters will be extremely slow, and any radionuclides leached from the canisters would stay with the immobile water in the rock pores. Such a concept requires a sound scientific basis and cannot be taken for granted. Hence, important hydrologic issues in this case pertain to the characterization, evaluation, and modeling of infiltration, percolation, and the partitioning of flow between matrix and fracture in the unsaturated zone above the repository.

Clay-rich rock is a transitional material, with properties intermediate between soil and hard rock. Its properties are sensitive to water content, behaving as brittle rock at low values of water content and as ductile soft material at high values. Clay formations are considered to be an option for hosting nuclear waste repositories because of their very low hydraulic conductivity and potential for self-sealing (of fractures or openings in clay). Clay minerals also provide good sorption capacity for the retardation of radionuclide transport. Undisturbed clay has such a low permeability that hydrology is not much of a concern. However, flow (H) through clays may occur in fractures formed during excavation and repository operation, on account of mechanical (M) deformation and ventilation drying, as well as thermal (T) input from the stored radioactive wastes. Thus, hydrologic (H) issues arise due to coupled THM processes [Tsang, 1987; Tsang *et al.*, 2012]. The T-induced and M-induced fractures are found in a so-called excavation damaged zone (EDZ) [Tsang *et al.*, 2005], which can be 1 or 2 m thick radially around a tunnel, and there is evidence that conducting fractures may be formed several meters into the rock ahead of the advancing excavation face. Further, under the influence of changes in mechanical stress or temperature, bedding planes and impurities in the clay formation may also become initiated to form flow conduits. However, these fractures may self-seal over a period of days, months, or years, because of the plasticity of clay.

As a result of the above discussions, in section 2, the focus with respect to hydrologic issues for a waste repository in crystalline rock will be mainly on flow and transport in saturated fractured rock from the repository to the biosphere. Those for unsaturated tuff (section 3) will be mainly on flow from the land surface through the unsaturated zone to the waste repository. For clay rock (section 4), the focus will be hydrologic issues that arise from coupled THM processes.

1.3. Challenging Factors Common to the Three Rock Types

A few special factors make the study of flow and solute transport for the evaluation of performance of a nuclear waste repository particularly challenging. First, the performance evaluation involves long-term predictions into hundreds of thousands or millions of years over distances on the order of one or several kilometers, assuming that the repository is situated about 500 m below the land surface. To achieve adequate confidence in such long-term predictions requires the assurance that first all relevant hydrologic and hydrochemical processes are accounted for, including slow processes that are normally insignificant for prediction over years or decades. For this effort, natural analogue studies can provide some useful information and confidence building [Mazurek *et al.*, 2008; Simmons and Stuckless, 2010; Alexander *et al.*, 2015]. Second, the geohydrologic structures over the kilometer area of interest also need to be identified and their flow properties characterized. Omission of a significant fault in the region, either subvertical or subhorizontal, can introduce a significant error in flow predictions. This leads to the need for advances in site characterization methods. Not only appropriate techniques need to be developed to detect and measure individual features at the site, but there is also a need for an integrated approach to site characterization, with joint analysis of

complementary multidisciplinary data, and the construction of site structural models with an adequate degree of detail and confidence.

Besides the demand for long-term predictions, safety assessment for a nuclear waste repository has a focus on predicting the migration of low concentrations of radionuclides, rather than the migration of the mean concentration contour of a radioactive contamination plume. The earliest arrival time of radioactive contamination is very sensitive to the heterogeneity of the flow system. Hence, a more rigorous and properly defined characterization of heterogeneity is needed, including development of new upscaling methods that preserve fast flow path features. Since it is impossible to know all the details of permeability heterogeneity, the prediction of solute transport would necessarily involve uncertainties. Quantification of such uncertainties for the predictive quantity at hand is an essential part of method development in flow and transport modeling.

A further challenging factor in the hydrology of a waste repository is that the permeability structure and hydrologic boundary conditions may not remain the same over the time frame of interest for safe disposal. This is because new fractures may be created, and existing fractures may change in their permeability, because of mechanical stress changes induced by excavation as well as thermal output from the radioactive waste stored in the repository. For northern countries, large mechanical stress changes with major changes in upper hydrologic boundary conditions may also occur due to the advance and retreat of glaciation that occur every 120,000 years. Similarly, hydrochemical changes may also occur that involve local solute precipitation or rock mineral dissolution, and these would change local flow permeability. Thus, coupling of thermal, mechanical, and chemical processes with hydrology has been an active area of research associated with nuclear waste repository development, and major progress has also been made in this field [Tsang, 1987, 1991a, 1999, 2009; Stephansson *et al.*, 1996; Hudson and Jing, 2013]. For Yucca Mountain, infiltration as the upper hydrologic boundary condition controls the percolation in the unsaturated zone and this boundary condition will not remain constant with time. The present arid conditions (interglacial climate) at Yucca Mountain can transition to moderate semiarid conditions (glacial-transition climate).

One way some of these special challenging factors are addressed has been through multiyear experiments in underground research laboratories (URLs). These are large underground tunnel-and-room systems at a depth of several hundred meters, similar to that of the planned waste repositories. They allow direct observations of the rock at depth, and investigation of rock fractures and other geological features not normally available in surface-based studies. Further, the scale of URLs is on the order of several hundreds of meters, providing the possibility of studying the characteristics and impact of rock heterogeneity up to an order of a kilometer or more. An overview of URLs in the world can be found in Blechschmidt and Vomvoris [2010]. To date, URLs have played an important role in obtaining data and information on thermal, hydraulic, mechanical, and hydrochemical rock properties at depths of interest for siting nuclear waste repositories.

In the following sections, advances in research of hydrologic issues over the last three or four decades will be presented in the context of the three different rock types. First, the main hydrologic issues related to flow and transport in fractured crystalline rock will be presented (section 2). The discussions will be fairly comprehensive, covering conceptual developments, experimental techniques and evaluation methods, field observation and experimental studies, numerical modeling development, validation issues, as well as integration of all the information toward predictive modeling. We hope that this section presents an overview of all the important aspects of hydrological research needed to address the challenging factors presented above. Although this comprehensive approach has also been taken in work for the unsaturated tuff and clay cases, it will not be reflected in the discussion of hydrologic issues for unsaturated tuff and for clays in sections 3 and 4, respectively. Rather, in these sections, the discussions will be limited to some main hydrologic issues related to their particular geological setting and characteristics. This is both to avoid repetition and to keep the paper to a reasonable length. Some general remarks will conclude the paper.

2. Hydrologic Issues Related to Nuclear Waste Repository in Crystalline Rocks

2.1. Background and Introduction to Crystalline Rock Issues

An intensive research program on crystalline rock waste repositories was started in Sweden in 1977, forced by new, very strict laws on disposal of nuclear waste. The Swedish program constituted an early start for studying fractured rock but was soon followed by Canada, Finland, Switzerland, and the U.S. Two early

Figure 1. Illustration of important phenomena for a high-level waste repository in fractured crystalline rock. From KBS-3 [1983].

safety analysis or performance assessments for deposition of nuclear waste in fractured rock were made in Sweden. They were called KBS-1 and KBS-2, published in 1977 and 1978, respectively. KBS-1 was for reprocessed vitrified waste; KBS-2 was for spent fuel without reprocessing. In both the studies, conventional flow and transport modeling underpinned by laboratory and field experiments were used. The fundamental concepts were based on the rock conceived as a homogeneous porous medium. Based on these performance assessments, two nuclear power plants in Sweden were allowed to start operation.

In 1983, a more detailed study and performance assessment for a repository for spent fuel was made that was used to obtain permission to start operation of two additional power plants. The repository was to use the KBS-3 [KBS-3, 1983] design, which at present is to be implemented in Sweden and Finland. Several new ideas and concepts were introduced. In addition to the recognition that flow in crystalline rock would be dominated by rock fractures, the rock matrix was now understood to be porous. This implies that solutes in flowing water in fractures could be strongly retarded by diffusion into the rock matrix pores and sorption on the mineral surfaces therein. This was shown to cause very large retardation of radionuclides, allowing many key nuclides to decay to insignificance [Neretnieks, 1980]. Further, from tracer tests in fractures and fracture networks, it was found that preferential paths could form, which could lead to much faster solute transport than that of the mean mass. The phenomenon was called channeling. It became increasingly clear that the residence time distribution (RTD) of solutes could not be described as a Fickian process, and that early arrival, which is very important for decaying radionuclides, could not reliably be described by the advection-dispersion equation (ADE) [Matheron and de Marsily, 1980; Neretnieks, 1983]. Another important question was how mass transfer takes place between the deposition hole and the seeping water in a fracture that intersects the deposition hole. The equivalent flow concept, Q_{eq} , was introduced to describe the rate of solute transport to and from the canister [Andersson et al., 1982; Neretnieks et al., 2010]. Also, highly conductive fracture zones were found to potentially contain fast pathways for the radionuclides.

Figure 1 shows flow paths in fractured rock, and the release and transport of solutes to and from a copper canister with spent fuel. The figure also illustrates channeling, matrix diffusion, and the presence of a fracture zone in a repository with canisters embedded in compacted bentonite clay, placed in vertical boreholes from drifts.

It was realized that there was a need to obtain flow and transport data from deeper lying rock than what could be done in and between deep boreholes from the surface. A joint Swedish-U.S. research cooperation was initiated in 1977 to investigate rock mechanical, hydrologic, and solute transport, as well as thermal processes, in fractured granitic rock within a deep-underground research laboratory (URL) at Stripa, in central Sweden. Also, what is called THMC coupling between thermal, hydraulic, mechanical, and chemical processes was a key object of study, because for the repositories, all these processes would be coupled in complex ways when considering the space and time scales that have to be covered. It was called the Stripa project [Witherspoon, 2000]. Subsequently, in Canada, Switzerland, Japan, France, and the U.S., URLs were also built in crystalline rock. In Sweden, another URL was built at Äspö when Stripa was closed in 1992. A review of these early URLs, together with more recent URLs in various countries, may be found in Blechschmidt and Vomvoris [2010].

In Sweden and Finland, studies in URLs, together with extensive laboratory and modeling work, culminated in two safety assessments [SR-Site, 2011; Posiva, 2012], which have been submitted to the authorities in support of applications to build underground repositories. In these safety assessments, the concept of multiple

barriers to radionuclide escape and release to the biosphere was applied. One important barrier is the long-lived copper canister containing the waste. The second barrier is the engineered buffer, such as compacted bentonite, emplaced between the copper canister in deposition tunnels and the rock. The rock is another major barrier, because it physically protects the repository and it limits the water flow rate through the repository. The hydrologic and hydrochemical evolution over very long times must be well understood, because copper canisters do not corrode in pure water but have to be protected from any oxygen, sulfide, or other corrosive agents that can be carried by the groundwater. The swelling properties of the compacted bentonite surrounding the canister are influenced by the water chemistry. Should a canister be breached, radionuclides carried by the seeping water may be carried to the biosphere. Radionuclides carried by the water are retarded by sorption and matrix diffusion, and many radionuclides may have time to decay to insignificance during their transport.

The retardation is influenced by water chemistry. The solubilities and sorption properties of many actinides are redox sensitive. They can be much more soluble and sorb less in oxic waters than in anoxic. It is therefore essential that the waters near the repository remain anoxic. A few anionic nuclides, e.g., the long-lived ^{129}I , are very soluble and do not sorb at all on the rock minerals. They travel with the velocity of groundwater save for some retardation caused by diffusion into stagnant waters in the rock matrix pores. Most actinides are cationic and sorb on the inner surfaces of the rock matrix and can be greatly retarded. In granitic rocks, colloid concentrations are very small and in practice do not influence nuclide transport.

In a rock mass with fractures and fracture zones, the water may encounter many different paths with different residence times and different retardation properties. The salinity exchange between the porous rock and the infiltrating fresh water changes the density of the water and influences the flow rates and flow paths. The impact of glaciation and deglaciation that will occur during the many hundred-thousand-year cycles must also be considered. To model these complex and intertwined processes, the rock around and in the vicinity of the repository must be well characterized hydraulically, as well as geomechanically and hydrochemically.

In the following subsections, hydrologic issues related to a waste repository in crystalline rock and their development are reviewed according to the following topics: (a) flow and solute transport in fracture rock, (b) characterization and parameterization of fractured rock properties, experimental techniques, and evaluation methods, (c) field observations and experimental studies, (d) rock matrix properties, (e) mathematical and numerical modeling approaches, (f) validation issues, and (g) integration for predictive modeling.

2.2. Flow and Solute Transport in Fractured Rock

Considerable effort has been devoted over the years to understanding what causes the spreading of a tracer carried by water, and how to model and quantify this in a way that can credibly be used for predictive purposes in the performance assessment of nuclear waste repositories. The hydrodynamic dispersion and residence time distributions, RTD, of solutes have been much studied over many decades and are of great importance for nuclear waste repositories. A short radionuclide residence time will allow the radionuclide to decay less. Therefore, the need to understand and quantify the underlying mechanisms for the RTD has been given much attention. Some of this work is briefly described below.

An overview of the transport processes along individual fractures can be found in *Bodin et al.* [2003a, 2003b]. Traditionally, dispersion has been modeled as a Fickian diffusion process. Although this seems to be reasonable for homogeneous porous media, it is found to lead to unexpected consequences in stratified and fractured media. In experiments in fractures and fracture networks, very often quite strong non-Fickian dispersion is found. *Matheron and de Marsily* [1980] showed the conditions and some examples of non-Fickian diffusion. *Neretnieks* [1983] showed that in stratified media with largely independent channels in fractured rock, the “dispersion coefficient” will increase with observation distance. This would invalidate the advection-dispersion equation, ADE, in which the dispersion coefficient D_m is taken as independent of flow path length. It was also shown that matrix diffusion causes a spreading of a tracer pulse than cannot be described by Fickian dispersion and can even totally dominate the spreading of a tracer pulse [*Rasmuson and Neretnieks*, 1981]. Compilations of dispersion coefficients evaluated from a large number of tracer tests in fractured rock over distances from centimeters to hundreds of meters show this non-Fickian dispersion effect [*Gelhar et al.*, 1992; *Neuman*, 1995].

Stratification or channeling is also found in laboratory measurements in natural fractures in cores [*Neretnieks et al.*, 1982; *Moreno et al.*, 1985; *Chesnut*, 1994]. Stratification can be caused by aperture variations, see for

example, *Hakami and Larsson* [1996], *Keller* [1997], and *Develi and Babadagli* [2015]. Such information has been used in the simulation of flow and transport in variable aperture fractures. It was shown that preferential pathways develop, with one or a few paths that carry by far most of the water [*Moreno et al.*, 1988, 1990; *Tsang and Tsang*, 1987, 1989; *Tsang and Neretnieks*, 1998]. *Odén et al.* [2008] discuss regional channelized transport in fractured media when matrix diffusion and linear sorption is also active. The impact of the presence of fast channels on radionuclide transport has been studied by (for example) *Rasmuson and Neretnieks* [1986]. The impact of channeling in networks of paths on solute transport is yet to be fully understood but it can potentially be beneficial to repository performance [*Neretnieks*, 2015].

It has also been found that the rate of mass transfer to or from an impermeable object, such as a clay-filled deposition hole in the flow path, can vary considerably, depending on how the channeled flow behaves [*Liu and Neretnieks*, 2006]. Also, the impact of the aperture-to-fracture-length relationship has been addressed by *Baghbanan and Jing* [2008]. It was recognized that the measured aperture statistics cannot capture trends over more than the size of the sample. Most available aperture data on single fractures are at relatively small scales of a meter or less; the behavior at larger scales remains unresolved to date. Neglecting longer-scale correlations would lead to a seeming homogenization of the properties over long distances. If there were different magnitudes of nested correlation lengths, or if the structures were fractal, dispersion would increase more than what Fickian modeling would predict [*Neuman*, 1995].

In fracture networks, preferential flow paths can also be caused by the presence of long fractures, connected fracture echelons, and fracture zones. This is supported by observations on large outcrops where fracture traces vary from very short to hundreds of meters, and where often smaller fractures can be arranged in echelons, forming very long, potentially hydraulically connected flow paths. The larger fractures can form long persistent rapid flow paths. On an even larger scale, fracture zones with widths of fraction of a meter up to many tens of meters, consisting of a denser network of smaller fractures, are found. Such zones can extend over several kilometers. Fracture orientations often come in groups, and some orientations can have more fractures and fractures of different length distributions than others. The size, orientation, and transmissivity distributions can lead to a tensorial property of the hydraulic conductivity [*Neuman and Federico*, 2003]. This will cause the dispersion also to be a tensorial property.

The fractal properties of fractures and fracture networks on all scales have been recognized and have attracted interest. *Doughty and Karazaki* [2002] studied how a hierarchically fractured network influenced the spreading of a tracer plume and found that it can strongly influence RTDs. *Guimera and Carrera* [2000] analyzed data from 90 tracer experiments performed in low-permeability fractured media and explored correlations among parameters controlling flow and transport. They found that the correlation between first arrival time and porosity is larger than for peak arrival. First arrival has specific importance for radionuclide migration, because it gives less time for decay. They also found that in many of the experiments, matrix diffusion had contributed considerably to the dispersion. *Hjerne et al.* [2009] compiled and analyzed 74 cross-hole tracer tests in granitoid rocks in Sweden, from six sites used to obtain data for simulations of waste repository performance assessment. Peclet numbers are reported to vary from 1 to 30 in single fractures and from 1 to 300 in fracture zones but show essentially no trend of increasing with distance. This implies that a Fickian dispersion coefficient would increase with travel distance. A large Peclet number indicates that the tracer pulse spreads little or moderately. A small Peclet number implies a large standard deviation of the RTD and suggests the presence of preferential pathways.

Berkowitz [2002] reviewed and analyzed measurements, conceptual pictures, and mathematical models of flow and transport phenomena in fractured rock systems. *Berkowitz et al.* [2002] discussed different conceptualizations of the underlying physical processes. *Neuman and Federico* [2003] discussed how different scales of experiments and observations can affect the interpretation of hydraulic tests. They concluded that for fractured rock, there are no generally accepted methods that would give unambiguous results. The multifaceted nature of hydrogeologic scaling is illustrated by a number of examples. *Molz et al.* [2004] discussed flow and solute transport in fractal fields in heterogeneous porous media, fractures, and fracture networks. They give an overview of measurements for the fractal properties of fracture surfaces and fracture apertures, as well as of fracture networks. They discuss the difficulties of obtaining data that can be used for extrapolation and prediction of flow and solute transport, as well as to validate models based on fractal and multifractal rock properties. *Fomin et al.* [2011] studied mass transport in the subsurface within a multiscale rock formation, which is constituted by porous domains dissected by the network of fractures. It was

modeled as a fractal medium, which resulted in fractional-order differential equations that exhibit anomalous diffusive mass transport. Berkowitz *et al.* [2006] developed a continuous time random walk method to model non-Fickian transport. Notwithstanding all the efforts described above, to date, no general, comprehensive method has been developed that can be used with confidence to predict dispersion in fractured rock masses using ADE-type equations.

The difficulties of modeling dispersion as a Fickian or modified Fickian process have stimulated development of stochastic discrete fracture network (DFN) models, in which one would track the paths of a multitude of particles. The idea is that this would obviate, or at least decrease, the need to include Fickian-based hydrodynamic dispersion. The differences in residence times would result in “dispersion.” In DFN models, the paths particles take are traced through the entire network. A choice is randomly made of which new fracture the particle would flow into at a fracture intersection. Along each path with individual properties, one can account for sorption, matrix diffusion, and other linear reaction processes that influence the RTD. The different mechanisms that contribute to dispersion are not lumped into a single entity, the dispersion coefficient. This is in stark contrast to what is done with ADE modeling.

Several models have been developed based on fracture networks and channel networks where the 3-D networks are generated stochastically using measured statistics on frequencies, sizes, orientations, transmissivities, and apertures of the individual fractures. The fractures are often assumed to be circular disks or rectangles. It is possible to calculate the flow pattern in each fracture, even if they have variable apertures, but then each fracture must be treated as a 2-D object. This is computationally very demanding in large networks [AMEC, 2014]. An early approach was to treat each fracture as a conduit, with a conductance derived from its transmissivity width, and some averaged length based on the distance between the intersections [Cacas *et al.*, 1990a, 1990b]. This is still done in network calculations with a large number of fractures. Along each path through the network, the outlet concentration from one fracture will contribute to the inlet concentration to the next fracture. The solute mass outflow from this path, at any given time, to a desired effluent point (or area), together with all other paths leading to this point, gives the total mass outflow and concentration as a function of time; i.e., the RTD. In the section on mathematical and numerical methods, the solute transport along a path is elaborated further.

2.3. Characterization and Parameterization of Fractured Rock Properties: Experimental Techniques and Evaluation Methods

In order to evaluate flow and solute transport in fractured rock, the characterization of geologic rock units and properties, geochemical properties of rock, large fracture zone extents and their properties, and orientations, sizes, transmissivities of general fracture networks are needed in considerable detail.

During the last decades, a number of different issues that influence flow and solute transport in fractured rocks have been identified and studied. A considerable number of papers have been published. We point to a few important overview papers. Berkowitz [2002] reviews methods and issues in characterizing flow and transport in fractured geological media. Neretnieks [2004] discusses the question of predicting solute transport in fractured rock, the models and processes and raises some concerns. de Marsily *et al.* [2005] discuss how to deal with heterogeneity. Neuman [2005] gives a detailed overview of the needs and challenges in characterizing the hydraulic properties of fractured rock on scales of what can be done by tracer tests and reviews the work that has been done in this area during the previous decades. Tsang [2005] and Tsang *et al.* [2008] discuss the issues connected with making long-term predictions. In this section, some of the experimental methods that have evolved over the last decades, stimulated by the needs of performance assessment of nuclear waste repositories, are briefly described. Some examples are presented for illustration.

Figure 2 shows a hydrologic conceptualization of the crystalline rock with deformation or fracture zones and less fractured rock between them. Using a large number of cored boreholes down to a kilometer and more, information is obtained on the different rock domains and major fracture zones. The latter are called hydraulic conductor domains (HCD). The less fractured rock between is called the hydraulic rock domain (HRD).

We will later discuss three different ways to conceptualize and model flow and transport in fractured rock masses. In the context of field measurement of important parameters, there is a need to mention briefly

Figure 2. Illustration of the principal features in the hydrogeological model from Rhén et al. [2003, Figure 3-2].

these models here. Besides modeling the rock as a continuum porous medium CPM, it can be modeled also as an equivalent stochastic CPM, called ECPM, in which the rock is modeled as consisting of a large number of usually small calculational elements each with different (but constant) hydraulic properties. In discrete fracture network (DFN) models, the rock is modeled as consisting of a 3-D network of connected conducting 2-D fractures. In channel network models (CNM), the conducting features in the rock are

modeled as “narrow” channels connected in a 3-D network. All three models will have the same flow porosity and flow-wetted surface per volume of rock. This ensures that the mean water residence time and the mean retardation of sorbing solutes will result in all models.

2.3.1. Hydraulic Conductivity/Transmissivity

Information on hydraulic conductivity K_h of the rock for use in equivalent porous media models and transmissivities of fractures for CNM and DFN models is a prerequisite for modeling of flow and transport in fractured rock. Several techniques are available for such measurements in boreholes. In packer tests, sections of the borehole are isolated by two or more inflatable packers. The isolated section is subjected to a hydraulic head higher or lower than the hydraulic head in the rock at the packer location, and the flow rate into or from the rock is recorded. The flow rate is used to assess the rock transmissivity in the isolated section. If the section contains only one fracture, this gives the fracture transmissivity. A large packer spacing would give information on some average hydraulic conductivity, which can be used in equivalent porous media ECPM modeling, elaborated upon later. Packers are also often used to measure hydraulic properties in fracture zones with very high intensities of flowing fractures.

Figure 3 gives an example of HRD and HCD data from the Laxemar site for packer tests with 100 m packer spacing [Rhén et al., 2008]. There is a clear decreasing trend with depth. However for a given depth, the data span over 5 orders of magnitude or more. The HCD conductivities are larger than HRD values by about 1 order of magnitude at repository depth. It is obvious that the rock is hydraulically very heterogeneous.

Packer tests are time consuming, and several more rapid techniques have been developed and used during the last decades. Impeller flow meters have long been used, however, with low accuracy. More sensitive

Figure 3. Hydraulic conductivity (K) for test scale 100 m versus elevation. K shown for test sections between major deformation zones (DZ) and test sections intersected by identified HCD's. Laxemar site [Rhén et al., 2008].

tools have been devised that are suited for rapid screening of deep boreholes in low-permeability rocks, such as those considered for deep repositories of nuclear waste. Two methods based on chemical or thermal tracer dilution are briefly described as follows. In the Posiva flow log method [Öhberg and Rouhiainen, 2000], a set of rubber discs is used at the two ends of the measurement probe to isolate the test section from the rest of the borehole. The length of the test section is typically 2 m. The discs will press themselves against the borehole wall and isolate a test section into which any water from a fracture intersecting the test section will enter. Its flow rate is derived from measuring the temperature change, or its rate of change, induced by a thermal pulse. The hydraulic head in the borehole is lowered and kept constant to induce the flow. The water above the upper end and below the lower end of the tool is allowed to flow unimpeded through a bypass tube of the section, and will not interfere with the flow rate in the test section. The flow from the test section leaves the monitoring tube above or at the bottom of the test section, depending on the flow direction (inflow or outflow). The significant advantage of isolating the test section with rubber discs instead of inflatable packers is that moving the tool from one test location to another takes place practically in a few minutes. Using several tests with two or more different hydraulic head drawdowns, the hydraulic head profile of the rock surrounding the borehole section can also be derived. With the Posiva flow log tool, individual fracture transmissivities lower than $10^{-9} \text{ m}^2/\text{s}$ can be obtained.

In the chemical dilution method, an idea similar to that described above, the electrical conductivity of the water flowing from all hydraulically conductive fractures into a borehole, under constant rate pumping, is monitored as it dilutes the fresh water with which the entire borehole fluid has been filled. The measurement involves scanning the whole length of borehole with a standard electric conductivity probe without the need of packers, rubber discs, or specially designed probes. This method, which is quite sensitive, also has the additional advantage of supplying information about the electrical conductivity or salinity of the water from different hydraulic fractures [Tsang *et al.*, 1990; Tsang and Doughty, 2003; Doughty *et al.*, 2013].

The location of each flowing fracture can be determined with an accuracy of a few tens of centimeters, even at depths down to a kilometer. This, together with detailed fracture mapping of the bore cores, is used to derive correlations between transmissivities on the one hand, and fracture orientations, depths, and other characteristics of the fractures, such as thickness of layers of secondary minerals on the other. An example may be found in the results of the two recent site investigations in Sweden at Laxemar and Forsmark. At these two sites, several tens of boreholes down to over 1000 m with nearly 100,000 individual fractures were characterized. Among all the fractures, only 2–3% had measurable transmissivities [Follin, 2008]. The transmissivity data from the Forsmark site can be represented by a semicorrelated transmissivity-fracture size model

$$T = 10^{ar^b + \sigma_{\log[T]} N[0,1]}$$

where T is the fracture transmissivity, r is the fracture radius, a and b are constants, and $N[0,1]$ denotes a normally distributed random deviate with a mean equal to 0 and a standard deviation of 1 [Joyce *et al.*, 2010].

2.3.2. Fracture Aperture, Fracture Coating, and Flow-Wetted Surface, FWS

Fracture aperture influences the water residence time. Fracture coating influences sorption and diffusional access to the porous rock matrix, and the flow-wetted surface (FWS) influences solute retardation and hence the residence time. Fractures have variable apertures and may contain crystal fragments and colloidal clay particles. Secondary minerals may coat the fracture surface and other precipitates; the original rock matrix near the surface may be mechanically disturbed when the fracture formed and may be also chemically altered in various ways. These alterations seldom extend more than a few millimeters, but on occasion can extend several centimeters in granitoid rocks [Löfgren and Sidborn, 2010]. The alterations are practically always as porous as, or more porous than the rock matrix at larger distances from the fracture face. For long times, when the diffusion has penetrated far beyond them, their presence can mostly be neglected. However, in tracer experiments with durations of less than a year or a decade, the properties of the altered zone can dominate or entirely determine the results, which makes extrapolation of tracer test to long times and distances very uncertain.

The mean fracture aperture available to in situ fracture flow can be assessed by tracer tests, provided the flow path dimensions are known or can be assessed [Guimera and Carrera, 2000; Hjerne *et al.*, 2009]. However, the results can be challenged, especially for longer experiments in which matrix diffusion dominates

the RTD. The use of the cubic law, which gives good results for constant aperture planar slits, gives a lower bound of the flow accessible, or mechanical aperture. A discussion of the different ways the fracture aperture is defined may be found in Tsang [1992].

In their compilation and analysis of 74 cross-hole tracer tests in granitoid rocks from six sites in Sweden, Hjerne *et al.* [2009] also report “mass balance apertures,” which has the same meaning as mechanical apertures in other publications, as function of transmissivities. These data can be used to estimate the mechanical aperture from transmissivity data, acknowledging that the uncertainty is considerable. No simple relation between mechanical and cubic law aperture has been found and up to order(s) of magnitude differences have been observed [Tsang, 1992].

It may be appropriate here to emphasize that the solute RTD is not only determined by the flowing water residence time, which is obtained from the mechanical aperture in the flow path, fracture width, and flow rate. In addition, the retardation caused by matrix diffusion must be accounted for. The flowing water residence time can be much smaller than the solute residence time in the stagnant water in the rock matrix. The latter is strongly influenced by the flow-wetted surface to flow rate ratio, A_q/q and the materials property group, $\varepsilon_p \sqrt{D_p R_d}$. A_q is the flow-wetted surface in a fracture(channel), q the flow rate, ε_p to rock matrix porosity, D_p the pore diffusion coefficient, and R_d the matrix retardation coefficient. These are central quantities for modeling of solute RDT in a flow path. For the long times and flow paths of interest here, the solute residence time is clearly dominated by matrix diffusion effects and is in practice independent of the flowing water RTD. This implies that the uncertainties in fracture aperture negligibly influence the solute RTD.

The fracture intensity is measured in boreholes that penetrate the rock mass and is denoted $P10$ in this paper, which has the meaning that, on average, $P10$ fractures are found per meter along the borehole. In a network of random fractures of different sizes and orientations, a thin borehole that intersects $P10$ fracture per meter gives the intensity of fractures in the rock. Fractures in which flow can be induced must be connected to the network of conductive fractures. $P10$ is independent of fracture size but can depend on their orientation in relation to the orientation of the borehole.

The flow-wetted surface (FWS) in the rock mass can be estimated from intensity $P10_{flow}$, (number of transmissive fractures per meter borehole) corrected for the fracture-intersection angle to the borehole by the Terzhagi correction. This correction takes into account the lower probability of fractures that intersect the borehole at an angle not perpendicular to the borehole. With the corrected intensity, the (mean) specific flow-wetted surface a_R of the rock is $a_R = 2 \times P10_{flow,corr} \frac{m^2_{surface}}{m^3_{rock}}$ as the fracture has two sides in contact with the flowing water. In equivalent continuum porous media models (ECPM), a_R determines the FWS in the rock volume considered. In fracture network models, each fracture has twice the FWS as the size of the fracture. In channel network models, where the channels have some average width W_{ch} and length L_{ch} , a sufficient number of channels must exist per volume of rock so that they together sum up to the observed $P10_{flow}$. More detailed discussion on how FWS in fractured rock can be assessed from measurements of $P10_{flow}$ can be found in Neretnieks [2015].

Channel widths cannot be determined with present-day methods from borehole measurements. Observations in tunnels and drifts of the widths of channels from which water flows can be used for this purpose. The channel surface density (CSD, number of channels per square meter exposed rock face) together with $P10_{flow}$ can also give estimates of channels widths. From this information in the same rock mass at a site, the width is $W_{ch} = P10_{flow,corr} / CSD$. One problem is that, of course, rarely does one have access to this information from a site at the depth of interest before drifts and tunnels have been excavated. So far, observations of channel widths from different sites have been used to estimate channels widths, which have been found to be between very narrow, essentially wormhole size, to tens of centimeters [Stanfors, 1987; Abelin *et al.*, 1991b, 1994; Tsang and Neretnieks, 1998]. Similar difficulties in obtaining important data are also present for the fracture network models, where fracture size distribution is based on observations of surface outcrops. This information also cannot be obtained from borehole data. There are also difficulties in getting such data from drifts and tunnels, because fractures larger than a few times the diameter of the drift tend to be truncated, unless they are essentially intersecting the drift along the drift orientation. There are thus several challenges remaining in using network models with some degree of confidence for modeling of solute transport over long times and distances.

2.3.3. Fracture Size Distributions

Fracture sizes, fracture size distributions, and orientations are needed for the DFN models. Fracture trace lengths are measured on outcrops and used to determine fracture sizes and distributions. Fracture trace

Figure 4. A set of fractures with closed and open regions intersected by a borehole.

length intensity is denoted P_{21} , (m trace length/m² area). The distribution of trace lengths is used to estimate fracture size distributions usually modeled as circular discs. Account is taken of the fact that trace lengths are always equal to or smaller than the diameter of circular fractures. In the Laxemar and Forsmark rocks, the fracture size distributions can be described by a truncated power law distribution, which includes data also for the fracture zones [Rhén et al., 2008]. The fracture sizes range from radii less than 10 cm to more than 100 m.

For illustration, some results are briefly summarized. In the detailed fracture investigations at Laxemar and Forsmark [Rhén et al., 2008; Rhén and Hartley, 2009], about 10% of the nearly 100,000 fractures inspected in detail on the cores were characterized as open or partly open. However, only 2–3% of all fractures had measurable transmissivity. At Laxemar, the Terzhagi corrected value for all fractures, P_{10} , ranged from 0.5 to 1 m⁻¹ at 50–150 m depth and were about a factor 10 lower at repository depth. At Forsmark, the intensity was considerably lower at repository depth.

Some fractures may be fully closed, but extremely few fractures can be fully open over their entire size, because the in situ rock stresses will tend to close them. Exceptions can be conceived in locations where the differential stress causes the rock parallel to the main stress component to force the crack to open. The connected open channels can conceivably exist more or less evenly distributed over all fractures or predominantly be present in some of them. The sum of the FWS in them must be the same, however, and equal to $a_R = 2P_{32_flow}$. Figure 4 illustrates the concept of channeling in fractures and how a borehole may intersect flowing and closed locations.

2.3.4. Fracture Zones

Fracture zones are present at different scales. Large zones can extend over many kilometers at depth and be many tens to hundreds of meters wide. They can often be seen on the ground, and their locations and orientations in the rock can be confirmed by boreholes. These large zones are treated as deterministic features in modeling. Smaller zones are often identified only in the boreholes, and their extent and orientation can sometimes be determined if they are intersected by several boreholes and if it can be ascertained that the same zone has indeed been intersected by the boreholes. The minor zones can be treated as stochastic features and incorporated in the DFN and CNM. The transmissivity of the larger zones can be many orders of magnitude larger than individual fractures, and the hydraulic conductivity within them can vary considerably over the thickness. To exemplify, at Laxemar, the Terzhagi corrected values for all fractures in the large fracture zone, P_{10} , ranged from 0.05 to 2 m⁻¹ [Rhén and Hartley, 2009].

2.4. Field Observations and Experiments on Channeling

There are many direct observations that flow in fractures is channelized. This has been observed in laboratory-scale fractures [Neretnieks et al., 1982; Moreno et al., 1985; Brown et al., 1998; Huber et al., 2012; Ishibashi et al., 2014; Develi and Babadagli, 2015]. There are also observations at larger scales that show distinct channeling [Abelin et al., 1983, 1985]. There are observations of channeling in large field experiments as well as on rock faces in drifts and tunnels [Abelin et al., 1994; Birgersson et al., 1992, 1993; Tsang and

Figure 5. Flow rate distribution in the Stripa 3-D experiment. From Abelin *et al.* [1991a].

Neretnieks, 1998; Palmquist and Stanfors, 1987; Stober and Bucher 2006; Ishibashi *et al.*, 2014]. It is also found that many of the channel intersections themselves can conduct water [Abelin *et al.*, 1991a]. Detailed mapping was also done in the Kymmen Tunnel [Palmquist and Stanfors, 1987]. The channel density seen on the tunnel walls varied considerably; most of the fractures did not have visible channels, and often there were only one or two channels in the more prominent, longer fractures. It was also noted that often considerable flow was found at fracture intersections. This is consistent with the observation in later laboratory experiments [Glass *et al.*, 2003] that preferential flow paths occur at fracture intersections.

Sparse boreholes cannot give information on the detailed spatial distribution of flowing channels, which would be very useful information for validating CNM and DFN models. An example of detailed flow rate distributions over a large area is from the so-called 3-D experiment in the Stripa URL. At 360 m depth, a 75 m long drift with a 25 m long crossing drift was covered with 375 plastic sheets, each 2 m² in size. Water flow rate to each sheet was collected for several years [Abelin *et al.*, 1991a, 1991b]. In the right part of Figure 5, it is seen that the water flow rates into the 375 plastic sheets cover a large span, one sheet taking 10% of the flow and 12 sheets taking 50% of the flow to the drift. It is also seen that large portions of the drift have no flow and that the flow paths/channels appear in clusters. The channel width behind the plastic sheets is not seen, but they are at most equal to size of the sheets.

The left part of Figure 5 shows the three vertical drill holes in which different tracers were injected in nine different points, 11–50 m above the drift. These tracers were collected in the plastic sheets over several years, and the BTCs were analyzed. The tracers were found in 175 different sheets in different proportions, sometimes bypassing paths taken by other tracers in the 3-D network of channels. This showed that a complex channel network was present on the scale 70 × 50 × 5 m. In this experiment, correlations were sought between flow rate, fracture intensity, orientations, and other observables, notably the intensity of fracture intersections (number per drift length). It was found that only the fracture-intersection intensity gave a clear correlation. Also, in other tunnels and drifts, fracture intersections have been observed to conduct water at considerable flow rates compared to the channels in the fracture plane.

In a smaller-scale dedicated channeling experiment also at Stripa, tracer transport over some meter distances in a “prominent” fracture was studied with a special “multipede” packer system. A complex channel network was found to exist outside the “prominent” fracture, as indicated by some of the injected tracers arriving at five different locations on the face of the drift wall outside the “prominent” fracture. These were in addition to flow paths in the “prominent” fracture, which was presumed to have practically all of the flow [Abelin *et al.*, 1994]. This was similar to the earlier findings in the 3-D experiment, but on a smaller scale. Unexpected flow paths in the rock outside a “prominent” fracture were also found in a third experiment, the 2-D experiment [Abelin *et al.*, 1983] and in the more recent TRUE experiment at the Äspö URL [Neretnieks and Moreno, 2003].

No systematic studies of channel widths have been made to date, nor have any measurement methods been tested to measure seepage rates below what can be measured by collecting dripping water. There

are, however, a number of direct observations that suggest widths of millimeters to decimeter sizes. Some surveys have tried to group the flow rates from channels in a few groups denoted by $<$, $<<$, and $<<<$ covering flow rate ranging from an occasional drop to frequent drops to small stream [Palmquist and Stanfors, 1987; Stanfors, 1987]. A survey of flow channels after excavation of the drifts and tunnels at Forsmark in Sweden, at depths of 50–100 m, reported more than 400 flowing channels over a total surveyed area of 14,000 m². The channel widths were reported to be up to about 20 cm. Flow rates, measured by collecting the dripping water, were found to vary from less than 0.1 to 5 L/min [Tsang and Neretnieks, 1998].

2.5. Rock Matrix Properties

2.5.1. Matrix Diffusion-Connected Porosity

Pores in the rock matrix are possibly connected over large distances but could also be connected over a short distance. In the latter case, only a limited volume of rock immediately adjacent to the fracture surface would be accessible to the solutes, and retardation would be limited. Considerable effort has been spent to study the connectivity of the matrix pore space, especially rock in situ that has not been destressed by taking and bringing samples up to the laboratory.

In the laboratory, diffusion properties are typically measured by subjecting the two opposite sides of a cylindrical core to a high solute concentration on one side and a low concentration on the other side, and then measuring the rate of solute transport through it. From the concentration breakthrough curve, the porosity, ε_p , of the sample can be determined as well as the pore diffusion coefficient D_p [Skagius and Neretnieks, 1986a].

The connectivity over distance is studied by using longer samples. Longer samples need experimental times that increase with the square of the sample length, which can lead to uncomfortably long experimental times. An alternative method is to fill the pores with an ionic solute containing simple salts, NaCl or NaI, and to measure the electric conductivity. Electric conductivity of a salt solution can be directly related to diffusivity by the Nernst-Einstein relation. The measurements are very rapid and are made with alternating current, AC, to avoid polarization effects. The saturation of the sample with the salt solution can take weeks or more with large samples. This in practice sets a limit to the size of the sample that can be used. Samples in the simple diffusion experiments are not subject to the stress that rock at depth is. Experiments with non-stressed and stressed samples have been performed, as both direct through-diffusion and electrical conductivity experiments [Skagius and Neretnieks, 1986a,b]. They show a decrease in diffusivity on the order of a factor 2–3 when subjected to stress similar to that at 500 m depth.

Techniques have also been developed with direct current, DC, to measure the continuous rate of transport of a salt through the sample. This is much faster than the through-diffusion experiments and gives comparable results with the previous mentioned methods. It additionally supplements the AC method as the ions migrate all the way through the sample and are not just oscillating, as in the AC method [André et al., 2008b].

The samples used in the laboratory have all been destressed compared to the rock stress under which they have been subject to for millions to billions of years. It thus cannot be ruled out that microscopic cracks between and within the crystals have formed by stress release during sampling, which irreversibly do not close when restressed in the laboratory. A study of diffusion in undisturbed rock in the field was undertaken at the Stripa URL at 360 m depth. A 20 cm diameter borehole was drilled from a drift to a depth of 15 m [Birgersson and Neretnieks, 1990]. This distance was about two drift diameters, and at such a distance, it is not expected that the presence of the drift would disturb the natural rock stress. From the bottom of the 20 cm borehole, a 20 mm diameter, 3 m long borehole was drilled. This was filled with a mixture of three solutes, packed off and pressurized to the measured hydraulic head at this location. Three such experiments were made. They were overcored after 3, 6, and 36 months, respectively, to retrieve the rock around the injection hole. In the 36 month experiment, several parallel boreholes also retrieved rock from distances up to 40 cm from the injection borehole. From the retrieved rock, 2500 samples were leached and analyzed for tracer content. The tracers were found at distances from 5 and up to 37 cm, showing that the rock had a connected porosity even under undisturbed natural stress.

Electrical conductivity methods to measure the diffusivity of the rock in deep boreholes have been developed and used in two sites in Sweden from several tens of meters up to 1 km deep boreholes that were

core drilled [Löfgren and Neretnieks, 2003]. The electrical conductivity is measured rapidly by a set of electrodes that send out the electrical current radially in a focused beam about 10 cm thick. Tens of thousands of measurements in the boreholes show that the porosity is connected over at least many meters, and that the diffusivity is of the same magnitude as is found in the laboratory, although somewhat lower due to the compression caused by the rock stress [Löfgren, 2007a,b]. These results are conveniently reported as formation factors F_r , which is the ratio of conductivity (diffusivity) of a sample and of water of the same shape. This information gives direct input to hydraulic and transport modeling [Rhén et al., 2008; Joyce et al., 2010].

2.5.2. Sorption

Crystalline rocks such as granitoid and gneissic rocks consist to a large extent of different aluminosilicates. They also contain other minor minerals, with iron, magnesium, calcium, and other metals as oxides, carbonates, or sulfides. The aluminum and silicon oxide mineral surfaces in contact with water can form surface hydroxyl, $\equiv OH$, groups, which can remain neutral. The symbol $\equiv$ stands for "attached to surface." Adding a proton, they become positively charged $\equiv OH_2^+$, or releasing a proton, they become negatively charged, $\equiv O^-$, depending on pH. In near-neutral waters such as normally found in deep groundwaters in granites, the surfaces normally have a surplus of negative charge. Common cations such as Na^+ and Ca^{2+} , as well as other positively charged ions, such as many radionuclides, can then attach to the negative surface groups and are sorbed by electrostatic forces. Other species, neutral or charged, can form surface complexes, which can be even stronger than electrostatic attachment. Compounds at trace concentrations increase their surface concentration in proportion to their concentration in the water. This is the basis for surface sorption coefficients K_a and mass sorption coefficients K_d . K_d is usually reported in unit of m^3/kg and will therefore also depend on how large a sorption area a mass of rock contains. K_d measurements are commonly made after crushing the rock to very small particles or even powder. This is necessary in order to decrease the equilibration time, because the sorbing species are retarded in their diffusion into the rock samples, and it may take years even for moderately sorbing species to equilibrate with a centimeter sized sample. Measurements on different sized particles are used to extrapolate to large samples. Such methods have weaknesses, because fresh surfaces are generated by crushing and grinding. Sorption on pieces of cores have been made by electro in-diffusion, but only for Cs, which has simple chemistry [André et al., 2008a, 2008b]. Measurements of the magnitude of sorption surface is made by nitrogen adsorption at low temperatures by the BET method on crushed rock, and the method has also recently been adapted to measurements on pieces of drill core [André et al., 2009]. Techniques for measuring sorption on noncrushed samples of redox sensitive elements and strongly sorbing species are still to be developed.

Negatively charged species will avoid the region nearest to the negatively charged crystal surfaces, and thus will not have access to the entire porosity, implying that their effective diffusivity will be smaller than for similar noncharged species [Retrock, 2004].

2.6. Mathematical and Numerical Approaches to Modeling of Flow and Solute Transport

In this section, some additional concepts and approaches of practical importance for solute transport modeling are described and discussed.

Darcy's law is used to model steady state flow rates in homogeneous, inhomogeneous, and fractured rock when the flow is laminar. The spatial distribution of flow rates in the rock calculated from either porous media or DFN models (or combinations thereof) is used to determine flow paths by particle tracking from potential locations in a nuclear waste repository to the ground surface-biosphere. For every flow path, the water residence time, flow rate, and the solute RTD can then be generated and used for dose calculations. Methods to calculate the RTD from flow path data are described below.

2.6.1. Porous Media and Reactive Solute Transport Modeling

The mathematical and numerical treatment of the advection-dispersion equation, ADE, applied to homogeneous and heterogeneous rock is often based on finite element, finite difference, or finite volume approaches, which can readily be done also for two-dimensional and three-dimensional problems, even when large numbers of chemically reactive species and matrix diffusion are to be accounted for. Steefel et al. [2014] present a general description of the mathematical and numerical formulations used in modern numerical reactive transport codes relevant for subsurface environmental simulations, including PHREEQC, HPx, PHT3D, OpenGeoSys (OGS), HYTEC, ORCHESTRA, TOUGHREACT, eSTOMP, HYDROGEOCHEM, CrunchFlow, MIN3P, and PFLOTRAN. These complex codes are used to calculate water flow and transport of solutes that react with each other and with rock minerals. They can in general handle porosity and permeability

Figure 6. Histogram of inflows to individual fractures given as rate of inflow per magnitude of drawdown. From *Rhén et al.* [2008, Figure 10–15].

changes in fractures and matrix. The codes are primarily aimed at complex geochemical calculations but can also handle flow in porous media. Several of these codes have been used to model the geochemical evolution of pore waters and seeping groundwaters. For large volumes of heterogeneous and fractured rock masses, they are less suited, because the computations become very time consuming, and very large computer memories are needed. Under certain circumstances, such codes can, however, be used even for complex 3-D flow fields in homogeneous media, if local-scale transverse dispersion/diffusion can be neglected between streamlines. This can be a reasonable approximation under strongly advection-dominated flow under steady state conditions. In this case, the flow field can be reduced to a set of streamlines that can be treated independently. In a homogenous medium, the flux-averaged concentration, and other quantities of interest at a given location, can be obtained by a single simulation of the evolution along one streamline that incorporates all the relevant geochemical processes (e.g., mineral dissolution/precipitation, aluminosilicates weathering, cation exchange reactions, and aqueous redox reactions). See for example, *Trinchero et al.* [2014].

For solute transport in fractured media where the only interaction between solute and rock is linear sorption, the CNM and DFN model approaches with particle tracking can be very effective. This is discussed below.

2.6.2. DFN Modeling

Stochastic discrete fracture network models have gained much attention since the pioneering work of *Long et al.* [1982]. The stochastic DFN networks are generated based on fracture intensity, transmissivity, and orientation data obtained from borehole and cores. Fracture size distributions are derived from fracture trace maps on outcrops. To ensure that the generated DFN model can reproduce the flow rate distributions measured in the boreholes, at least stochastically, flow rate distribution simulations are made and compared with those observed in the boreholes. The procedure, which is rather complex, is described in *Rhén et al.* [2008]. An example of such comparison from the Laxemar site for the rock at depths between -650 and -400 m is given in Figure 6.

In the DFN model, each transmissive fracture is typically assumed to have the same transmissivity over its plane. However, it is accepted that this cannot be true, and one important question is how channeling affects the magnitude of the FWS that the water flowing in a fracture contacts. *Larsson et al.* [2012] studied what fraction of the fracture surface area the water that flows in a fracture will be in contact with, as a function of the logarithm of transmissivity and correlation length of the transmissivity distribution over the fracture. They present the results as the specific flow-wetted surface sFWS as a function of the fraction of total flow through the fracture. An example is that for a standard deviation of the log conductivity of $\sigma_{\ln K} = 4.61$ and a correlation length of 6% of the fracture size, 80% of the flow is found to be in contact with less than 10% of the fracture surface. Then this fraction of the flowing water has $A_q/q = 0.125$ of the average in the fracture. This can have a considerable impact on the retardation in the fracture. *Larsson et al.* [2013] showed how sFWS can be included in DFN modeling.

In DFN models with evenly transmissive fractures, the fracture intersections exhibit no resistance in the flow direction but allow no flow along the intersection. When variable aperture fractures modeled with discrete elements intersect each other, the flow rate from one element in a fracture to the opposing element in the other fracture will be strongly influenced by the element with the smaller transmissivity. If, however, the fracture intersections are assumed to have large transmissivity, then the most transmissive path from the delivering fracture will be well connected to the most transmissive path in the receiving fracture. This does not seem to have been included in the DFN models but has been included in the channel network model (CNM) [Moreno and Neretnieks, 1991, 1993; Gylling, 1997; Gylling *et al.*, 1999]. The channel network model also has two other noteworthy differences from DFN models, in which matrix diffusion is assumed to be linear and orthogonal to the fracture surfaces. First, a channel in a fracture, may be in contact with stagnant water in the fracture plane into which solutes may also diffuse, and second, in narrow channels, the diffusion will become increasingly cylindrical around the channels as the diffusion depth becomes as large or larger than the channel width. This leads to more rapid access to larger matrix volumes and causes increased retardation [Neretnieks, 2015]. The effect can be very large when the channels are narrow.

2.6.3. Hybrid Approach and the ECPM

Discrete fracture network models tend to become very demanding on computer resources. Hybrid approaches have been developed in which fine meshes capable of handling very detailed regions are imbedded in coarse meshes that can cover large rock volumes (where the need for high resolution is less). Several approaches are combined [e.g., Cacas *et al.*, 1990a, 1990b; Tsang *et al.*, 1996; Niemi *et al.*, 2000; Öhman *et al.*, 2005; Svensson *et al.*, 2010], and they often include calculating block-scale properties with a fracture network model and then using these block-scale values in a stochastic equivalent continuum model at the larger scale. At an even larger scale, where there is no need for accurate particle tracking, deterministic porous medium modeling can be used. The data needed for the equivalent continuum porous model (ECPM) can be obtained by measuring the rock mass conductivity in boreholes using, for example, packer tests with packer interval set to a distance similar to the block sizes to be used in a stochastic ECPM model. Another way to obtain the data for the ECPM is to make a multitude of DFN simulations with the block sizes of interest, and then to determine the hydraulic conductivity tensor of the equivalent porous medium blocks. An exploration of this technique was made by Niemi *et al.* [2000], who also discuss the uncertainties of this approach.

In the hybrid approach, major fracture zones can also, if desired, be included using ECPMs derived from the zone properties. The detailed network models can then be used only in the regions where very high resolution of the detailed flow is needed, e.g., where there are local contaminant sources (such as damaged waste canisters) from which the release rate depends on local flow rate past the individual waste canister.

In the Swedish and Finnish repositories based on the KBS-3 design, many thousands of canisters are spread out over about 1 km², and each can be treated individually [SR-Site, 2011; Posiva, 2012]. A network model is used for the immediate repository region, but the more distant rock covering a much larger volume can be modeled as a porous medium, based on the ECPM properties derived from stochastic simulations of rock volumes ranging from 20³ to 100³ m³ with DFN structures. The stochastic simulations yield direction-dependent hydraulic conductivity and FWS in the block. The inner DFN region and the outer ECPM region are then coupled and solved simultaneously to generate a very large number of particle tracks, which can then be used for solute transport modeling. This mixed technique, as used in the recent Swedish performance assessment of the proposed spent fuel repository at Forsmark in Sweden, is described by Rhén *et al.* [2008].

2.6.4. Modeling Impact of Sorption and Matrix Diffusion Along a Flow Path

Radionuclides will have trace concentrations and sorption that can be modeled as a linear and reversible process. The solute transport equations are then linear—a situation that can be used to make important simplifications, compared to when, for example, precipitation/dissolution reactions occur and complex non-linear geochemical codes must be used. A short outline of a procedure for this situation is given below. A more detailed description of the method can be found in Retrock [2004].

If one can identify flow path sections with constant properties (such as in a single fracture/channel/conduit), a very simple equation describes the concentration evolution along the path over time exists for the case where only advection and matrix diffusion need be considered. The output from one fracture gives the input to one or more fractures at the next intersection by convolution. Using the Laplace transform method,

which eliminates time, the output from the N th consecutive fracture in a flow path can be found as a product of the input concentration to the first fracture, multiplied by a product of the N equations for each fracture along the flow path. Each fracture may have different flow rates and properties. Numerical inversion gives back the dependence on time. Examples can be found in *Cvetkovic et al.* [2004], *Neretnieks* [2006a], and *Cvetkovic and Frampton* [2012]. Different paths consist of different numbers of conduits, and most of the conduits are likely different. This method is fast: thousands to tens of thousands of paths can readily be computed on a desktop computer. Long radionuclide decay chains can also be treated in this way [*Neretnieks*, 2006b]. The conduits wherein the flowing water is in contact with the rock matrix (as described above) can have more complex additional mechanisms and properties. One example is the presence of practically stagnant water zones in the fracture itself adjacent to the flowing channels. The solute may then also diffuse in to these regions, from which in turn it can diffuse into the matrix [*Neretnieks*, 2006a; *Mahmoudzadeh et al.*, 2013]. This results in additional retardation. The presence of different layers of coatings and alteration zones on the fracture surface also influences the exchange of solutes between flowing water and rock. The coatings can have different porosities, diffusion coefficients, and sorption properties, as well as increased or decreased retardation. Analytical solutions in Laplace space have been obtained also for this case. Further, radionuclide decay chains can be directly incorporated in CNM [*Mahmoudzadeh et al.*, 2014].

The Laplace-transform-based methods cannot be used when properties and conditions change over time, such as changes in flow rates or of sorption properties caused by changes in water chemistry. Particle tracking techniques have been developed and adapted to such conditions using a method called *time domain particle tracking* [*Painter et al.*, 2008; *Painter and Mancillas*, 2009]. In principle, it stops the particle at a point in time when conditions change and resumes the particle tracking with the new conditions from the location at which the particle was stopped. It has been used in the MARFA code [*Painter and Mancillas*, 2009] and has been successfully compared to solutions obtained by the Laplace-based method. It has been applied to long-term flow rate and direction changes caused by glaciation and deglaciation scenarios [*Selroos et al.*, 2013].

Matrix diffusion can also have a strong impact on the chemistry of the water seeping in the fractures and indirectly on the water flow rate and direction. The exchange of salts between the seeping water and the matrix pore water influences the density of the flowing water and causes buoyancy effects. Fresh meteoric water that infiltrates the fracture network in the rock, which may have old salt water in the matrix, will increasingly pick up out-diffusing salt from the matrix. This can have a considerable influence on its flow rates and directions. It can also influence the sorption of solutes via the sorption coefficients, which change with chemical composition of the water. With traditional finite elements or similar methods, one can model these changes but the discretization tends to become prohibitive. *Carrera et al.* [1998] developed a method that avoids the discretization of the rock matrix by use of a “memory function.” This has successfully been incorporated in the main code, ConnectFlow, used by SKB [*SR-Site*, 2011].

2.6.5. Modeling RTD in Fracture Zones

Fracture zones can in principle also be modeled as fracture networks. This, on the one hand, would lead to an additional very large network, and on the other hand demand a detailed characterization of their properties. Fracture zones at present are treated as homogeneous or heterogeneous porous media, and they are assumed to have very little retardation. An alternative to this treatment has been proposed based on the notion that a fracture zone consists of porous blocks and particles of different sizes. A simplified conceptual picture of block size distributions in fracture zones can be formalized in a mathematical model that accounts for the block size distribution, as well the different shapes of the block. *Neretnieks and Rasmuson* [1984] used a pseudobody concept that captures these effects, showing that this could be incorporated without penalty to computation effort. *Rasmuson* [1985] derived a solution for solute transport through a medium with blocks of variable size, shape, and properties. Transport in fracture zones has not been addressed in detail in recent modeling for performance assessment of nuclear waste repositories, probably because there have not been many detailed characterization and data-collection efforts of the fracture zone properties in the field. If the rock fragment size distribution in the HCD can be better characterized, their retardation potential could be better utilized. However, the potential presence of fast and persistent channels in the HCDs adds to the uncertainty. All these may well be good reasons to make closer studies of solute transport in HCD.

2.7. Validation Issues

For deep geologic repositories of radioactive wastes, it is not possible to perform experiments that cover the distances and time scales of interest to demonstrate that the repository isolation capability is sufficiently

good. Thus, it is a major challenge to try to “validate” modeling results of flow and solute transport over the distances and long time scales to achieve a sufficient confidence level. An intensive effort has been made to attempt to build chains of evidence, based on fundamental laws of nature, to show that the most dangerous escaping radionuclides from the repository will have time enough to decay to insignificance before they reach the biosphere. All processes involved are fundamentally simple and well understood, but knowledge of the geology and the rock structures at a given site at various scales can vary considerably. It is not possible with present-day tools and methods to identify and describe in detail all possible flow paths and their properties. Often simplifications, such as homogenization, must be made in representing hydrogeological structures, especially small-scale features, when conducting solute transport modeling. Tsang [1991b, 2005] discusses the different roles of processes and structures in model validation and emphasize the need of uncertainty quantification and assessment.

In striving for general model validation, many of the key processes and mechanisms have been experimentally validated in experiments ranging from small-scale laboratory to large-scale field tests over years and even decades. In addition, observations of natural processes that have been active over long times and distances can be used to support the predictive modeling. Some field-scale experimental techniques and experiments are briefly described below, as well as some natural analogues that are used to support the arguments that the models used to capture all reasonable uncertainties.

2.7.1. Chemical Imprint of Groundwater Transport Over Long Times

One approach to gain more confidence in predicting the long-term evolution of groundwater chemistry is to attempt to reproduce the composition of present groundwater and matrix pore water that is extracted from deep boreholes and cores. The chemical characteristics of a water sample can be based on concentration of major ions—such as the cations Na^+ , Ca^{2+} , Mg^{2+} and anions Cl^- , CO_3^{2-} , SO_4^{2-} —and their concentration ratios. These signatures are used to derive information regarding deep saline groundwater mixing with recent meteoric water. In Scandinavia, the imprint of the seawater of the Littorina Sea, which existed 7500–4000 years BP in the region where the Baltic sea is at present, is also used. This sea contained brackish water distinctly different from that of present-day Baltic water [Laaksoharju *et al.*, 2008]. The results of mixing calculations have been compared or integrated with hydrodynamic models. Even if the original groundwater compositions of the mixing members are not known in detail, it is possible to estimate them by the mixing calculations, which can give further confidence in the results [Carrera *et al.*, 2004].

Trace elements of radionuclides ^3H , ^{14}C , ^{36}Cl , can give information on water residence times and migration mechanisms. Tritium, ^3H , with a half-life of 12.33 years, was produced in large quantities during the 1960s by hydrogen bomb tests in the atmosphere. Peak concentrations in rainwater reached nearly 6000 tritium units (TU) compared to ~ 5 TU by natural production in the atmosphere. This implies that if groundwater samples contain more than a few TU, the mean water travel time to the sampling point is less than ~ 50 years. ^{14}C has a half-life of 5730 years but is more complex to use in studying water travel time, because it participates in precipitation/dissolutions reactions. Cosmogenic ^{36}Cl has a half-life of 301,000 years and its absence in deep groundwaters indicates that these have not been admixed with meteoric water over very long times. Concentration profiles of dissolved ^4He , which is constantly produced by uranium and thorium in crystalline rocks, and migrates by molecular diffusion from large depths, have been used to demonstrate that the rate of transport by advection at depths below some hundreds of meters is very low, and that groundwaters have been essentially isolated for millions of years [Neretnieks, 2013; Kietäväinen *et al.*, 2014]. The ratios of $^2\text{H}/\text{H}$ and $^{18}\text{O}/^{16}\text{O}$ and $^{87}\text{Sr}/^{86}\text{Sr}$ in the groundwater and minerals give information on the temperature of the water that precipitated and infiltrated as groundwater, and on the time when secondary minerals were formed. This can also be used to indicate if the infiltration occurred during an ice age or during a warmer period [Drake *et al.*, 2012]. Such information can be used as an argument that a very large fraction of the water at repository depth has not been mobile over a million year time scale. It does not prove, however, that a small portion of the water cannot reach the biosphere in a shorter time.

2.7.2. Natural Analogues

There have been great expectations that observations of imprints of natural processes could be used to verify, even quantitatively, hydrologic and transport processes over long times and distances; see for example, Miller *et al.* [1994]. For hydrologic purposes, quantitative comparisons have rarely been successful, because initial and boundary conditions have seldom been possible to ascertain with sufficient confidence. Evidence of retardation by reversible sorption has also proved to be difficult, because of the reversibility of any accumulation of a solute. In contrast, evidence for matrix diffusion of irreversibly reaction solutes is found in the

context of ore formation. Although it has not been possible to directly use *quantitative* information from natural analogue studies in performance assessments for nuclear waste repositories the studies have qualitatively confirmed that the different processes in the models exist in nature and that the observations do not contradict the modeling.

2.7.3. Tracer Tests

Numerous tracer tests have been made, ranging from laboratory-scale to field-scale tests, over hundreds of meters and up to a kilometer scale in crystalline rocks. A large number of such experiments have been evaluated [Guimera and Carrera, 2000]. The tests have had various aims, including process understanding and validation, obtaining field data for use in predictive models, and supporting modeling in performance assessment studies for nuclear waste repositories. Summaries and overviews of such tests and how they can be used in support of predictive modeling can be found in Moreno and Crawford [2009] and Löfgren *et al.* [2007]. The main findings of these reports are that field-scale tracer tests can confirm flow connectivity and can confirm the existence of solute retardation, but they alone can only broadly substantiate our process understanding. Field-scale tracer tests might ideally deliver the product of the material property group and the FWS to flow rate ratio, but they alone cannot deliver individual transport parameters, such as effective diffusivity, or specific flow-wetted surface. Lumped or individual transport parameters obtained from inverse modeling of tracer test data are not transferable to PA flow conditions or time scales. Detailed reasons for these findings are presented and discussed by Moreno and Crawford [2009]. Some of the main reasons they give are that, as the results show, radionuclide transport in such tests and performance assessment, while governed by the same retardation mechanisms, are dominated by different subprocesses at different times. Parameter values, typically fracture apertures and in situ apparent retardation data, determined in tracer tests, should not be used directly for making PA predictions.

2.8. Integration of Mechanisms, Processes, Observations, and Field and Laboratory Data for Predictive Modeling

The above-described concepts, models, approaches, data, and more were brought together to assess the escape of radionuclides to the biosphere from a repository in a fractured crystalline rock in Sweden and Finland. In this work, it became increasingly clear that a strictly consistent description was needed. Hydrologic issues played a prominent role, and all modeling had to be supported by geologic, hydrologic, and hydrochemical field observations, which must be interpreted to support the models on all scales. Contradictory information must be resolved, and prediction uncertainties quantified, when possible. A short description of how this was done is presented below, with references given to a few of the main underlying reports from the Swedish program.

The objective of the *SR-Site* [2011] study was to assess the long-term safety of a KBS-3 type repository located at Forsmark in northern Uppland, Sweden. A similar project was carried out in Finland [Posiva, 2012]. Follin *et al.* [2008] describe the hydrogeological conceptual model and numerical modeling using the ConnectFlow code. The impact of stress on the hydraulic properties of fractured rock has been studied by Min *et al.* [2004], and Follin and Stigsson [2014] describe a transmissivity model for deformation (fracture) zones and its possible correlation to in situ stress. Hartley and Roberts [2012] describe discrete fracture network modeling as applied to hydrogeology of the Forsmark and Laxemar sites. Hartley and Joyce [2013] describe approaches and algorithms for groundwater flow modeling in support of site investigations and safety assessment of the Forsmark site.

Selroos and Follin [2014a,b] give an overview of the site descriptive model for the proposed site, and the same authors provided, in a previous report [Selroos and Follin, 2009], an integrated description of all hydrogeological modeling conducted, as well as an outline and summary of how the *SR-Site* groundwater flow modeling and radionuclide transport was performed. They go on to describe the hydrogeological modeling strategy and model setups used for *SR-Site*, specifically how the different time periods, scales, and model tools relate to each other. They provide a rationale for the hydrogeological base cases and variants defined for the different hydrogeological model applications as well as an evaluation and discussion of the results obtained in the different hydrogeological model applications performed. They point out that while hydrogeology within safety assessment applications traditionally has been focused on delivering data and conditions for use within transport calculations of radionuclides, the hydrogeological analyses within *SR-Site* additionally devote particular attention to the evolution of hydrogeochemical conditions in the geosphere driven by changes in the climate and surface system. This is because hydrogeochemical conditions in the

bedrock have a significant bearing on the long-term performance of the buffer in a waste repository. Hence, the geosphere needs to be assessed, both in terms of its effect on the engineered barriers and its own performance as a barrier. *Crawford* [2008] describes how the bedrock transport properties were obtained and parameterized based on laboratory and field data. *Follin et al.* [2014] describe how confirmatory testing of a groundwater flow model was made.

More detailed and in-depth descriptions of the flow and transport modeling is reported in a paper by *Joyce et al.* [2014] who have used the ECPM coupled to CPM and DFN models to enable modeling the hydrology and radionuclide transport at Forsmark in Sweden.

2.9. Concluding Remarks to Crystalline Rock Issues

Site characterization will be a cardinal enterprise underlying any modeling of water flow and solute transport in fractured rock. For prediction of solute transport, more detailed information is needed than for prediction of water fluxes [Tsang, 2005]. This is especially important when chemically active solutes are of interest. Reasonably rapid and accurate methods have been developed to assess the flow-wetted surface and matrix diffusive properties, but the structure of flow paths is more uncertain. Most notably, the potential presence of persistent flow paths with more than average flow rates, in which the solute is exposed to limited retardation, is not practically possible to detect with present methods. Such long-range channeling effects could have an important impact on predictions of toxic or radioactive compounds. This may well be one of the major uncertainties.

Channel widths cannot be determined from borehole measurements and underground facilities must be used where direct observations can be made on drift and tunnel walls. Reliable techniques have yet to be developed. Because diffusion from narrow channels tends to become radial with time, this can considerably increase the retardation of solutes compared to linear diffusion, which has been invariably used in modeling up to now. Channel widths also impact the density of channels in the channel network, which together with potential for radial diffusion also influences retardation.

Validation of solute transport models against in situ traces tests may not be applicable to long-term predictions, because man-made tests over distances longer than hundreds of meters and over more than 10 years would be extremely difficult to perform, and even so would only cover a limited number of pathways [Neuman, 2005]. The problem is further aggravated by the presence of altered rock matrix near the fracture surface, which changes matrix diffusion and sorption properties, and also the presence of fracture coatings and infill. The tracer RTD from short-term tests is determined by the surface material near the fracture, but the long-term RTD is dominated by the properties of the underlying rock.

Boreholes used to characterize a site are very sparse spatially, implying that few fractures and minor fracture zones will be intersected by more than one borehole. A systematic study on the uncertainties caused by the sparseness of information on solute transport might help to quantify the uncertainties.

We summarize the main findings that were stimulated by the need for predicting radionuclide transport in fractured crystalline rocks as follows. Solute transport in fractured rocks has been the main hydrologic problem of interest for nuclear waste repositories and has stimulated experimental and theoretical studies that have led to new insights. The enormous importance of diffusion in the porous rock matrix was identified around 1980. It had scarcely attracted any attention previously. This stimulated the development of methods to quantify the flow-wetted surface over which the solute exchange between mobile water in fractures and stagnant water in the matrix occurs. Laboratory and field techniques to determine the rock matrix properties that influence diffusion in the matrix and sorption on the inner surfaces of the rock matrix were also developed. The question of possible fast paths in which nuclides may not have ample time to decay raised serious challenges of the commonly used advection-dispersion equation and led to the development of fracture and channels network models, which was made possible with new information of flowing fracture/channel frequency obtained in boreholes with new equipment of high spatial and transmissivity resolution. The use of groundwater composition data from many locations at depth in the study area to validate flow and transport models has evolved along two lines. First, mixing proportions of meteoric waters, deep saline waters, and relic waters from the latest ice age have been used to verify models of movement of water masses. Second, geochemical models coupled to hydrologic transport models were developed and shown to be able to predict evolution of pH and redox conditions. This has been used to demonstrate that

the buffer capacity of the rock minerals is sufficient to eliminate penetration of chemical pulses to large depths; a crucial question, as this might severely influence the solubility and migration rate of many of the highly toxic redox sensitive actinides.

3. Hydrologic Issues Related to a Nuclear Waste Repository in Unsaturated Zone in Tuff

3.1. Background and Introduction to Unsaturated Rock Issues

Compared to nuclear waste disposal programs in countries where geological disposal will be in saturated rocks below the water table, Yucca Mountain, which was proposed at one time as a potential repository site in the U.S., is unique, in that the proposed repository would be located in unsaturated rock approximately 300 m above the water table in a thick (~500–750 m), unsaturated zone of volcanic tuff [Dyer and Voegelé, 1996; Snyder and Carr, 1982; Buesch *et al.*, 1996]. Winograd [1974] first proposed storing nuclear waste in the unsaturated zone, and in a later paper Winograd [1981] pointed out the perceived assets of waste disposal in a thick unsaturated zone, including extremely low flux of water in the unsaturated zone under arid and semiarid climatic conditions, and the high sorptive capacity for radionuclides in valley-fill sediments, which commonly occur in the unsaturated zone.

The main attribute of the unsaturated zone—the limited availability of water that could come in contact with waste (and thus initiate transport of radionuclides)—played a paramount role in the safety strategy at the Yucca Mountain. A main pillar of the safety strategy was that if little or no water were to enter into the emplacement drifts that house the waste canisters, to corrode them and to expose and dissolve the waste, then the consideration of fate and transport of radionuclides becomes inconsequential, since the source term of transport has already been dispensed with. This rationale drives the site characterization and modeling studies at Yucca Mountain to emphasize gaining a sufficient understanding of how water moves in the unsaturated zone, and particularly in the unsaturated zone above the waste-emplacement drifts. The emphasis is to affirm whether the natural barrier in fact protects the emplaced waste from being contacted by water. The processes that control water movement through the unsaturated zone to the repository horizon will be (1) climate and precipitation, (2) net infiltration, and (3) percolation. These stand in considerable contrast to the hydrological focus for repositories in the saturated zone, which centers on the transport of radionuclides in the geologic formation from the waste canisters to the biosphere.

Before we launch into these hydrological issues, which comprise the subject of this section, we first provide some background on the disposal program in the U.S., as related to Yucca Mountain. The United States national policy for the disposition of high-level radioactive waste and commercial spent nuclear fuel was established by the Nuclear Waste Policy Act of 1982. In 1987, Congress amended the Nuclear Waste Policy Act, directing the Department of Energy to characterize only the Yucca Mountain site. In 2008, in culmination of almost three decades of investigations at Yucca Mountain, the Department of Energy completed a Safety Analysis Report as the License Application [USDOE, 2008a,b] to the United States Nuclear Regulatory Commission for authorization to construct a waste repository at Yucca Mountain. Although the U.S. subsequently (in 2010) changed its plans so as to pursue alternative solutions to a radioactive waste repository at Yucca Mountain, the Nuclear Regulatory Commission nonetheless published the evaluation report by its staff on the subject of safety after permanent closure at Yucca Mountain [USNRC, 2014]. The report concluded that, with reasonable expectation, the Department of Energy has demonstrated compliance with the Nuclear Regulatory Commission regulatory requirements for postclosure safety.

Yucca Mountain may be one of a few most extensively and thoroughly studied geologic features on earth. The documentation of the investigation at Yucca Mountain leading to the license application in 2008 is sizable, in the form of many project reports, journal literature, and conference proceedings. Since in this present paper, we shall have a narrow scope, discussing only a few important hydrological issues, it seems appropriate that we provide in the following some literature references indicating the broad coverage this topic received, along with a comprehensive bibliography. In a special issue of *Reliability Engineering and System Safety* [2014] entitled “Performance assessment for the proposed high-level radioactive waste repository at Yucca Mountain,” the authors attempt to provide a reasonably complete and accessible description of the proposed Yucca Mountain repository, from initial concept to the performance assessment that supported the 2008 license application. According to the guest editorial [Helton *et al.*, 2014], the papers in this special

issue are divided into two groups. The first 10 papers are primarily of a historical nature, but with a substantial technical content, and describe the investigations and analyses performed for the Yucca Mountain site from 1978 through 2008. The second group of 15 papers provides a detailed summary of both the structure of the 2008 Yucca Mountain performance assessment and the results obtained from the safety analyses. Of most relevance to the subject of the present paper will be three papers in the first group on site characterization [Rechard *et al.*, 2014a], unsaturated zone modeling [Rechard *et al.*, 2014b] and transport modeling [Rechard *et al.*, 2014c]. The extensive reference lists in the papers in this special issue demonstrate the scale of investigation that was undertaken at Yucca Mountain and can serve as a valuable resource to the general scientific community.

Prior to the 2008 submittal of the license application, the Department of Energy was also required by Federal regulations to prepare a document entitled "The Yucca Mountain Site Description" [USDOE, 2004]. This regulatory document is a compilation of more than 20 years of scientific research with the resulting understanding of the geology and hydrogeology of the Yucca Mountain Site. Evolved from the work originally reported in the Yucca Mountain Site Description, scientists at the United States Geological Survey, and at the Department of Energy National Laboratories, authored two companion volumes of monographs: Geological Society of America memoirs 199 and 209. The first memoir, edited by Stuckless and Levich [2007], summarizes the current understanding of the geology and climatology (past, present, and future) of the Yucca Mountain area. The second memoir, edited by Stuckless [2012], summarizes the understanding of the hydrology and geochemistry of the Yucca Mountain area. The different chapters in the latter memoir deal with the following subjects: (1) hydrology of the unsaturated zone [LeCain and Stuckless, 2012]; (2) the saturated zone hydrology [Belcher *et al.*, 2012]; (3) fluid geochemistry [Marshall *et al.*, 2012]; (4) the paleohydrology of unsaturated and saturated zones [Paces and Whelan, 2012]; (5) conditions and processes affecting radionuclide transport [Simmons and Neymark, 2012], and (6) effects of coupled processes on the proposed repository [Tsang, 2012]. Each chapter provides a rather comprehensive review of the science in its respective subject. We believe that the references in these chapters are an excellent resource for interested readers.

Because aridity is crucial to the isolation of radioactive waste in the unsaturated zone, repositories in the unsaturated zone seem inherently more vulnerable to climate change and water table rise than repositories located in the saturated zone. Based on the hypothesis that estimates of future climate conditions can be made by comparison to comparable conditions in the past, a great deal of effort has been expended to understand past glacial/interglacial cycles, how precipitation and infiltration rates changed with major climate shifts, and the effect of these climate shifts on water levels [see Forester *et al.*, 1999].

3.2. Hydrologic Setting and Important Hydrologic Issues

The stratigraphy of Yucca Mountain consists of laterally continuous, alternating layers of welded and nonwelded volcanic tuffs [Scott and Bonk, 1984], dipping gently to the east as a result of several high-angle faults. The welded tuff and nonwelded tuff have vastly different hydrological properties. The welded tuffs are characterized by relatively low matrix porosity (averaging ~ 0.1) and low matrix permeability (averaging $\sim 10^{-17} \text{ m}^2$), but high fracture density; while the nonwelded tuffs have higher matrix porosity (averaging 0.3) and permeability (averaging 10^{-14} m^2), but low fracture densities.

On the basis of the degree of welding, or subsequently on the degree of fracturing, the volcanic rocks in the unsaturated zone at Yucca Mountain are grouped into five hydrogeologic units [Montazer and Wilson, 1984; Ortiz *et al.*, 1985]. Beginning from the land surface, they are (1) the Tiva Canyon welded (TCw) unit, (2) the Paintbrush nonwelded (PTn) unit, (3) the Topopah Spring welded (TSw) unit, within which lies the repository horizon, (4) the Calico Hills nonwelded (CHn) unit, and (5) the Crater Flat group undifferentiated (CFu) units. The design of the proposed repository at Yucca Mountain assumed that the waste canisters would be emplaced in underground drifts of 5 m in diameter, within the TSw unit.

Figure 7 shows a schematic of the hydrologic issues related to the disposal at Yucca Mountain. The figure shows water flow reaching the repository horizon from the land surface and seeping into the 5 m diameter drifts, illustrating the hydrologic processes of: (1) net infiltration, the penetration of water below the zone of evapotranspiration and (2) percolation, the downward penetration of water through the unsaturated zone. The percolation patterns may be discontinuous through the welded fractured units TCw and TSw, and controlled by the fracture-matrix interaction in the unsaturated zone. In the porous nonwelded PTn unit, the

Figure 7. A schematic of the hydrologic issues related to the disposal at Yucca Mountain.

flow is likely continuous, and because of the tilting of the tuff layers, there may be lateral diversion of flow into faults.

Once the percolation reaches the repository horizon, one needs to understand the seepage of water into the waste-emplacement drifts since the opening in unsaturated zone provides a capillary barrier to the water flow [Philip, 1989; Philip *et al.*, 1989]. Furthermore, the repository design at Yucca Mountain entails that the near-field temperature is expected to rise above boiling for hundreds of years; therefore, the coupled thermal, hydrological, chemical, and mechanical processes with multiphase flow must also be addressed.

Figure 7 also indicates the hydrological issues below the emplacement drifts. Were the waste canisters within the emplacement drifts to become corroded by the water that had seeped into the drifts and the waste dissolved subsequently, then the transport of radionuclides comes into play. Because the drift, acting as a capillary barrier, diverts percolating water around it, this greatly reduces water flux immediately below the drift opening, thus significantly limiting the mobility of radionuclides. This is termed the “drift shadow” effect in Figure 7. Perched water bodies below the repository horizon illustrated in Figure 7 arise from the interface of more permeable nonwelded vitric tuffs underlain by impermeable zeolitic tuffs. These will have an effect on the percolation pattern to the water table. Below the water table in the saturated zone, sorption and matrix diffusion are the key factors retarding radionuclide transport.

For this paper, we have chosen to limit our discussion to a few of the important hydrologic issues illustrated in Figure 7; specifically, the issues for the unsaturated zone. In the following subsections, we shall address infiltration, percolation, and fracture-matrix interaction, and then end with a discussion of a three-dimensional numerical model which integrates moisture, pneumatic, thermal, and geochemical field data to study the flow pattern in the unsaturated zone.

3.3. Infiltration Flux Estimates

Of the average precipitation (about 170 mm yr^{-1}) [Hevisi *et al.*, 1992] in the Yucca Mountain area, most is lost to runoff and evapotranspiration. Between 1984 and 1993, the infiltration studies at Yucca Mountain

were conducted by monitoring of changes in water-content profiles in response to precipitation and snow-melt events by neutron logging in 99 shallow boreholes [Flint and Flint, 1995]. The studies show that second to precipitation, the depth of soil (alluvium) cover is most significant in controlling net infiltration. Measurements indicate that when the soil-bedrock contact reaches near-saturated conditions, fracture flow is initiated in the bedrock, increasing the hydraulic conductivity by several orders of magnitude. Soils exceeding 5 m in depth virtually eliminates the penetration of water into the soil-bedrock contact, except in the active channels that can collect and concentrate the runoffs.

Water mass balance calculations from precipitation, evapotranspiration, run-on, and runoff along washes were incorporated into a numerical model to develop a net infiltration map using average annual precipitation [Flint *et al.*, 2001a]. Map results show an average net infiltration of 2.9 mm yr^{-1} flux over the Yucca Mountain study area ($\sim 40 \text{ km}^2$) and 4.5 mm yr^{-1} over the potential repository footprint ($\sim 5 \text{ km}^2$). Temporally, no infiltration may occur for several years, and then $10\text{--}20 \text{ mm yr}^{-1}$, spatially averaged, may occur within 1 year. Spatially, no infiltration will occur where soil thickness exceeds 5 m, but where soil cover is thin, evaporation is low, elevation is high, and underlying bedrock is permeable, the net infiltration can be as high as 250 mm yr^{-1} .

Pore water chloride concentrations data from over 10 boreholes in the unsaturated zone had also been used for infiltration estimates. The pore water samples were extracted by uniaxial or triaxial compression from the nonwelded units [Yang *et al.*, 1996, 1998], and by ultracentrifugation from the densely welded units [Yang *et al.*, 1990]. Infiltration estimates were made based on the chloride mass balance approach [e.g., Allison and Hughes, 1978; Dettinger, 1989], assuming an average precipitation of 170 mm yr^{-1} , with an average chloride concentration of 0.35 mg/L . Since the measured pore water chloride concentrations spanned a wide range, resultant net infiltration estimates range from less than 0.1 to 10 mm yr^{-1} for a variety of topographic settings [Flint *et al.*, 2002]. The spatial variability of these estimates is consistent with findings derived from the moisture neutron log that thick alluvium cover is an effective barrier to water movement.

3.4. Percolation Flux Estimates

Percolation flux is defined as total vertical-liquid mass flux through both fractures and matrix and is converted to millimeters per year (mm/yr) per unit area using a constant water density.

Temperature data have been collected from more than 40 boreholes in the unsaturated zone at Yucca Mountain [Sass *et al.*, 1988; Rousseau *et al.*, 1999]. Based on the collected temperature and thermal conductivity data, Sass *et al.* [1988] estimated the heat flux and found a significant heat flux deficit. They attributed the deficit to energy uptake by water percolating through the mountain. Rousseau *et al.* [1999] applied a conductive and convective numerical model to temperature data from two boreholes and found significant variability in the inferred percolation flux. One advantage of estimating percolation flux by temperatures is that this approach is insensitive to the partitioning of the total percolation flux between fractures and matrix, which is uncertain, and an important issue to be discussed in the next section 3.5.

Bodvarsson *et al.* [2003], employing both an analytical solution for conductive and convective heat flux and a numerical model, performed an analysis of all the temperature data for all the boreholes. The analysis was performed with a five layer model, using measured core thermal properties [Brodsky *et al.*, 1997] for the respective alternating welded and nonwelded layers. The calculated temperature profiles were sensitive to the assumed magnitude of percolation flux, and the magnitude of the estimated percolation fluxes from the analytical solution compared well with that from the numerical simulations for all boreholes tested. The estimated percolation flux ranges from 0 to 20 mm yr^{-1} for most of the deep boreholes. The use of temperature data for the estimation of percolation flux is subject to a greater uncertainty for shallow boreholes, because temperature profiles can be affected by large gas flow. The fact that estimated percolation fluxes for boreholes at or near faults were generally higher than for the other boreholes could also arise from the temperature data being affected by gas flow in the faults.

3.5. Fracture-Matrix Interaction

3.5.1. Conceptual Models

Since the mid-1990s, flow through the unsaturated welded tuff at Yucca Mountain has been modeled by a dual-permeability approach, which treats the matrix and fractures each as a continuum; in other words,

both continua can conduct fluid, and nonequilibrium is allowed between the matrix and fracture continua. Numerically, dual permeability is implemented by representing each discretized rock volume by one fracture grid block overlapping and interacting with one matrix grid block. The area through which fracture-matrix flow occurs is traditionally calculated based on the geometry of the fracture network, assuming that flow occurs through all the fractures and is uniformly distributed over the entire fracture area. To model highly transient flow and transport between fractures and matrix, a refinement of the dual-permeability approach is made in which the matrix is further subdivided into several continua, depending on the distance to the fracture-matrix interface. This refined approach can more accurately resolve sharp gradients near the interface. This model was proposed by *Pruess and Narasimhan* [1985] and known as the multiple interacting continua (MINC) model.

However, for almost 10 years prior, it was commonly believed that liquid flow occurred predominantly in the matrix in the unsaturated fractured-welded tuff unit TSw [*Flint et al.*, 2001b]. This belief was based on the concept of capillary equilibrium between the fracture-matrix continua, and the fact that because of the fine pore size in the welded matrix (a few to tens of μm) [*Blair et al.*, 1984; *Flint*, 1998], the capillary suction was much stronger in the welded matrix than in the fractures. Since it was also accepted knowledge in soil physics that as the water-phase pressure in a porous medium was reduced below the atmospheric pressure, the largest pores would desaturate first, followed by the desaturation of successively smaller pores, then it seemed natural to infer that the fractures in a fractured porous medium would tend to remain dry under conditions of partial saturation, and that water would be held by capillarity in the finer pores of the matrix.

Based on this conceptual model, *Wang and Narasimhan* [1985] showed by a numerical study of flow through rock matrix with discrete fractures that flow in fractures could only be initiated or sustained when the matrix was fully saturated, that the larger aperture portions of the fractures remained dry, and that water flow between adjacent matrix blocks occurred only across fracture asperities. Thus, according to *Wang and Narasimhan* [1985], fracture flow in the unsaturated welded tuff occurs only under transient conditions during flooding near the land surface, which probably describes the rapid flow of infiltrating water in the topmost welded layer, TCw. Below TCw, the nonwelded layer PTn, having few fractures, would buffer and redistribute the infiltration flux, so that liquid flow arriving at the top of the welded repository layer TSw would be rather uniform and steady. Hence, based on the fracture-matrix interaction model of *Wang and Narasimhan* [1985], fracture flow in the TSw unit would be negligible.

Yet field evidence indicates the presence of fracture flow in the repository welded unit TSw. For example, secondary mineral deposits of opal and calcite present in fractures and lithophysal cavities of welded tuff indicate past pathways of water percolating through the unsaturated zone. Studies of secondary calcite and opal at the Yucca Mountain [*Paces et al.*, 2001; *Whelan et al.*, 2002] were initially based on samples from surface-based boreholes, and after 1995, on higher-quality samples within the Exploratory Studies Facility. The Exploratory Studies Facility was an 8 km long tunnel, excavated between 1994 and 1997, which provided underground access to the tuff layers for a series of field tests. The studies on rock samples showed that water with solutes percolating through unsaturated zone welded tuffs had formed a 1–40 mm thick secondary mineral coating on fracture footwalls or lithophysal-cavity floors, but these coatings were found in less than 10% of fractures and cavities examined.

Also, the unsaturated zone pore waters were found to be geochemically different from those in the saturated zone and perched waters [*Yang et al.*, 1996, 1998] below the repository level. The chemical differences were attributed to the mechanism that pore waters flow primarily through the rock matrix, whereas perched water accumulates primarily from flow through the fractures. For perched waters, isotopic data [*Paces et al.*, 2002] suggest that the flux of water through fractures is likely episodic and of small volume compared to the hydraulic conductivity of the fracture. Note that the fracture continuum permeability values in the welded tuff average about 10^{-12} m^2 , as derived from air injection tests that had been conducted extensively, both in surface-based boreholes and in the Exploratory Studies Facility [e.g., *LeCain*, 1997; *Cook*, 2000], while the matrix permeability values in the welded tuff average about 10^{-17} m^2 , based on laboratory measurements on cores [*Flint*, 1998].

A more compelling argument for flow occurring in fractures in the repository unit TSw is that the hydraulic conductivity of the matrix in the welded tuff simply cannot accommodate the estimated infiltration fluxes (section 3.3) without becoming fully saturated. Assuming a unit gradient liquid-phase hydraulic potential,

the maximum water flow rate through the matrix is the matrix hydraulic conductivity. The average matrix permeability in the fractured-welded tuff on the order 10^{-17} m^2 is equivalent to a hydraulic conductivity of less than 1 mm yr^{-1} . Then, the balance of the “measured” infiltration flux must be conducted by the fractures. To allow global flow in both the fracture and matrix continua requires a dual-permeability conceptual model.

In the 1990s, when the dual-permeability approach was first applied to the flow in the fractured-welded tuff, it was found that one could not utilize the full fracture-matrix interface area in the numerical implementation of fracture-matrix flow. A fracture-matrix interface reduction factor was needed in order to allow enough flux to flow through the fracture continuum without saturating the matrix continuum [Altman *et al.*, 1996; Ho, 1997; Bandurraga and Bodvarsson, 1999].

Though the fracture-matrix interface area reduction factor resulted in a good match between simulation results and the observed data on matrix water saturation and water potential data [Bandurraga and Bodvarsson, 1999], it was empirical and not rigorously derived. Therefore, Liu *et al.* [1998] proposed a new formulation for fracture-matrix interaction within the dual-permeability approach, based on the hypothesis that not all connected fractures actively conduct water in the unsaturated zone. They argued that even as fingering flow could occur in homogeneous unsaturated soils because of gravitational instability, so could gravity-dominated, nonequilibrium preferential liquid water flow bypass a portion of fractures, though the active and inactive fractures may have the same hydraulic characteristics, except for the presence of liquid water flow.

Liu *et al.* [1998] defined f_a , the fraction of fractures in the fracture network that are active in conducting water, as a power function of the effective water saturation, S_e , of the fracture continuum; that is

$$f_a = S_e^\gamma \quad (1)$$

where γ is a positive constant depending on properties of the corresponding fracture network, and the effective water saturation in connected fractures, S_e has the usual definition in terms of the fracture water saturation for all the connected fractures, S_f , and the residual fracture saturation, s_r

$$S_e = \frac{S_f - s_r}{1 - s_r} \quad (2)$$

If both the active fractures and inactive fractures are assumed to have the same residual saturation, then the effective water saturation of the active fracture S_{ae} is related to the effective saturation of the connected fractures, S_e , by

$$S_{ae} = \frac{S_e}{f_a} = S_e^{1-\gamma} \quad (3)$$

In the traditional continuum approach, the capillary pressures and the relative permeability characteristic curves are expressed in terms of the effective water saturation of all the fractures, S_e . In the active fracture model, S_e can be replaced by S_{ae} , the effective saturation of the active fractures, to obtain the capillary pressure relation for the fracture continuum. As for relative permeability, the liquid-phase relative permeability for the active fracture continuum is directly determined by the effective water saturation of active fractures and can be obtained by the substitution of S_e with S_{ae} . However, because only a portion of the fractures are active, the relative permeability of the entire fracture continuum should be the relative permeability of active fractures multiplied by the fraction of active fractures, f_a . So by the definitions of the above three equations, Liu *et al.* [1998] introduced one additional parameter, γ , into the traditional continuum characteristic curves where all fractures conduct water.

Since γ in the active fracture model inherently represents a large-scale process, the γ values cannot be determined by laboratory measurements of fracture core samples. Liu *et al.* [1998] inferred the γ values through inverse modeling using the site-scale unsaturated model (discussed in the next section, section 3.6) and field-scale data collected at Yucca Mountain. Their simulation showed that about 18–27% of the connected fractures are active, and average active fracture spacing is about 1 m in the TSw unit under ambient conditions.

This active fracture concept of the dual-permeability model has been incorporated into the large-scale transport numerical model for the unsaturated zone at Yucca Mountain [Robinson *et al.*, 2012a, 2012b],

which accounts also for all other major transport processes including radionuclide sorption and colloidal transport.

3.5.2. Field Testing of Fracture-Matrix Interaction

Many tests of different scales were performed in the alcoves, niches, and tunnels in the Exploratory Studies Facility to investigate issues important to the safe disposal at Yucca Mountain, such as percolation flow paths, seepage into drifts, and coupled processes (for a summary, see *Wang and Bodvarsson* [2003]). Observations of fracture liquid flow paths and seepage processes above niches [*Wang et al.*, 1999] had motivated additional tests in fractured-welded tuff to evaluate the contribution of rock matrix to overall flow and tracer transport. We discuss in the following three tests associated with fracture-matrix interaction in unsaturated welded fractured tuff.

Liquid release tests were carried out in a 2 m scale test bed in the TSw fractured tuff to evaluate the dominance of fracture flow and the dependence of flow on liquid release rates [*Salve et al.*, 2002]. The field experiment involved multiple release of tracer-laced water in two packed sections of a horizontal injection borehole, over a 6 week period. Two localized injection zones were selected based on their permeability values (2.7×10^{-13} and 6.7×10^{-12} m²) which were obtained by air injection tests [*Cook*, 2000] conducted in 0.3 m sections all along the borehole. During and after water release, the moisture wetting-front movement and the flow field evolution were continuously monitored in three monitoring boreholes. An excavated slot below the injection and monitoring boreholes was used to collect the fracture flow component that was not imbibed into the matrix. Collection trays in the excavated slot had 28 compartments, so the water collected in the trays could be quantified for volume, rates, and spatial locations.

Test results from injection into the lower permeability zone suggested flow through a highly heterogeneous fracture network in which the high-permeability fractures were not well connected or extensive. For liquid release into the higher permeability injection zone, about 60–80% of the release liquid was collected in the excavated slot in a matter of minutes, indicating high-conductivity well-connected flow paths. Furthermore, the arrival of the liquid at the slot was localized in only a few compartments of the collection trays, suggesting that flow predominantly occurred in preferential, channelized pathways, the “fast paths” commonly associated with partially saturated high-conductivity fractured rock [*Su et al.*, 1999; *Pruess*, 1999].

To simulate large infiltration events associated with El Niño conditions of high precipitation and to evaluate matrix effects over long flow paths, a large-scale infiltration test was conducted in Alcove 1 (about 5.5 m high and 5.8 m wide), in the TCw unit of the Exploratory Studies Facility, from 1998 to 2000. In this test, a drip irrigation system on the outcrop ~30 m directly above Alcove 1 was used. Water was applied uniformly over an infiltration plot of 7.9×10.6 m. The collection system in Alcove 1 consisted of 432 relative small trays placed just below the ceiling of alcove and was able to collect water from the entire ceiling of the alcove.

The infiltration test consisted of two phases. Duration of Phase I was 175 days, and the first arrival of water into Alcove 1 was on Day 57. In Phase II, a tracer was introduced into the infiltrating water. *H. H. Liu et al.* [2003] applied the active fracture model coupled with the MINC approach (section 3.5.1) to model this large-scale infiltration and transport test. The seepage data collected during Phase I of the test were used for model calibration by adjusting rock parameters, including porosities, permeabilities, and van Genuchten parameters for the relative permeability and capillary pressure characteristic curves [*Van Genuchten*, 1980], for both the matrix and fracture continua, as well as the active fracture parameter γ . The calibrated parameters were then used for model prediction of the Phase II test results. Comparison between experimental and modeling results showed that the continuum approach captured important features of flow and transport processes and also indicated that matrix diffusion may have a significant effect on overall transport behavior in unsaturated fractured rock.

Another large-scale infiltration and matrix diffusion test was carried out in the Exploratory Studies Facility TSw unit with improved testing approach and control. *Salve* [2005] presented the observations of preferential flow during the liquid release part of the experiment. The in situ field experiment involved the release of ~22 m³ of ponded water (at a pressure head of ~0.04 m) over a period of 7 months, directly onto a 12 m² infiltration plot located on a fractured-welded tuff surface. An array of horizontal boreholes, at vertical distances of 19 and 22 m below the infiltration pond, was instrumented with specially designed sensors to detect the arrival and persistence of flow through fractured rock. Note the different testing approach used

in this test from that of the small-scale test described earlier [Salve *et al.*, 2002] where water was injected into a localized borehole section.

Measured infiltration rates indicate that most of the water infiltrated through a limited section of the ponded surface, suggesting that partitioning of the ponded water into specific flow zones was initiated at this upper boundary. Distinct flow zones, with varying flow velocity, wetted cross-sectional area, and extent of lateral movement, intercepted the monitoring boreholes. There was also evidence of water being diverted above the ceiling of a niche (~ 4 m wide and 3.25 m high) in the immediate vicinity of the monitoring boreholes.

Observations from this field experiment suggest that isolated conduits, each encompassing a large number of fractures, develop within the fractured rock formation to form preferential flow paths that would persist if there is a continuous supply of water. The inclusion of numerous fractures in individual flow conduits suggests that the area across which fracture-matrix interactions occur may be significantly greater than would be expected from a model of focused flow along a fracture, which fits well the results of the smaller-scale liquid release test [Salve *et al.*, 2002]. This underlines the importance of field investigations at different spatial scales in order to provide data critical to the fundamental understanding of unsaturated flow in fractured rock.

3.6. Integrated Modeling

Figure 7 on the hydrological issues related to the disposal at Yucca Mountain shows the importance of the unsaturated zone flow patterns to the performance of the repository. Section 3.4 describes how the magnitude of an average percolation flux was estimated. However, to analyze and arrive at a quantitative pattern of the percolation flux poses a great challenge. It is not possible to quantify the flow paths on the spatial and temporal scales of interest to a waste repository by means of field measurements. Because numerical modeling offers a complementary means to study physical processes on scales not accessible to measurements, there was a sustained effort to develop three-dimensional mountain-scale flow models for Yucca Mountain [Wittwer *et al.*, 1995; Bandurraga *et al.*, 1997; Wu *et al.*, 1999, 2004, 2007]. The outcome of this effort was an integrated modeling methodology, which can be considered as an important advance in the hydrological science. This integrated approach attempted to incorporate as much data as were measured at Yucca Mountain, into one single three-dimensional numerical model. The diverse categories of data include hydrological, pneumatic, geochemical, and thermal. These were incorporated into one single model with the aim to provide percolation flux patterns and flow behavior. We shall give a brief summary of this integrated unsaturated zone model.

The aerial domain of the unsaturated zone model encompasses the Yucca Mountain study area, approximately 40 km². The three-dimensional discretization is of unstructured irregular grid blocks with a refined mesh in the vicinity of the proposed repository (~ 5 km²) near the center of the model. The model grid preserves the important large geological features: layers and near-vertical faults. Thus, the five alternative welded and nonwelded tuff tilting layers above the water table were explicitly represented in the three-dimensional numerical model discretization. The faults were represented by vertical or inclined 30 m wide zones. The model grid consisted of 2042 columns, each with both fracture and matrix continua, together with 59 computational grid layers on the average in the vertical direction, resulting in approximately 250,000 grid blocks and 1,000,000 connections in a dual-permeability grid.

The land surface and the water table were, respectively, the upper and lower boundaries of the model. The spatially distributed infiltration map derived from measurements as described in section 3.3 was applied as the upper boundary condition for the model. The numerical code used for this model was TOUGH2 [Pruess, 1991], which uses an integrated finite difference method and multidimensional geometry to calculate coupled flow and transport of air, water, and heat flow.

3.6.1. Model Input Parameters and Model Calibration in 1-D

To model unsaturated flow of water and air in a dual-permeability model, relative permeability and capillary pressure characteristic curves were the necessary inputs for both the fracture and matrix continua. For the mountain-scale flow model, the van Genuchten models of relative permeability and capillary pressure functions [Van Genuchten, 1980] were used to describe variably saturated flow in both fracture and matrix media, in addition to the active fracture parameter, γ for fracture-matrix interaction. Furthermore, other intrinsic fracture and matrix properties such as porosity, permeability, density, and fracture geometric

parameters, as well as rock thermal properties also served as inputs. As implied in the discussion in the previous sections, a considerable amount of field data had been obtained from outcrop samples, tens of boreholes, and underground tunnels in the Exploratory Studies Facility. These field and laboratory data constrained the assignment of input rock properties to the different hydrological units in the 3-D unsaturated zone model.

Model calibration to refine the input parameter as measured was performed in one dimension using the inverse modeling numerical code ITOUGH [Finsterle, 1999]. The model calibrations rely on field-measured data such as matrix-liquid saturation, water potential, temperature, perched water, and pneumatic data. The first step in the 1-D calibration was to extract the discretized columns from the 3-D model for those boreholes with the relevant calibration data. For example, for calibration against the combined measured data of matrix saturation and water potential, simultaneous inversions were performed on five 1-D columns [Bandurraga and Bodvarsson, 1999], while calibration against the pneumatic data [Ahlers *et al.*, 1999] involved 1-D columns for over 10 boreholes. In the inversion exercise, the goodness of fit between the simulated versus the calibration data was measured using a least squares approach.

Understandably, different input parameters would be sensitive to different types of calibration data in the inversion. The variations in the calibration parameters during the inversion were constrained by the standard deviations of the input parameters. The rock matrix input parameters generally were obtained from numerous direct laboratory measurements. Fracture input parameters were mostly derived from theoretical analyses using air-permeability measurements and fracture-mapping data. Thus, the allowed fracture parameter variance was set generally larger than that of the measured matrix parameter. The calibration in 1-D was concluded when the resultant parameter set provided a good fit to all the measured calibrated data in 1-D columns containing the calibrating data.

3.6.2. 3-D Simulations and Further Calibration

The parameter set estimated through a series of one-dimensional model inversion served as input parameters for the 3-D model. Further adjustment of some of the matrix and fracture input parameters was to be expected, since by the very nature of 1-D calibration, large-scale three-dimension flow processes were not accounted for. For example, some high-gas-flux channels may exist through faults or highly fractured zones. Therefore, by comparing simulated pneumatic results in the forward simulations in 3-D once more to the measured pneumatic data, slight adjustments were made to fracture permeability parameters of some modeled units to yield a better match to the pneumatic data. This was done for data from the approximately 10 boreholes that had been instrumented for passive pressure monitoring [Ahlers *et al.*, 1999; Wu *et al.*, 2007].

Another process in a 3-D model that would be absent in 1-D column simulations would be lateral diversion of liquid in the tilted nonwelded layer. Further calibration and confirmation was carried out in 3-D. The step of further calibration was similar to that described in the previous paragraph. By comparison of the water potential and matrix-liquid saturation results from 3-D forward simulations to the same water potential and matrix-liquid saturation calibration data previously used in the 1-D calibration, adjustments were made to the matrix and fracture property input parameters for improved match. Then, a second step of confirmation was carried out by tracer transport simulations of chloride based on the 3-D flow model with the updated input parameters. This was done because water percolation and infiltration flux history may be revealed in the study of geochemical data from the unsaturated zone [J. Liu *et al.*, 2003]. A comparison of simulated tracer transport results with chlorine concentration data collected in boreholes and Exploratory Studies Facility showed that the data set that provided the best match was also the data set that produced considerable lateral flow in the nonwelded layer (PTn) above the repository welded layer (TSw) [Wu *et al.*, 2004].

3.6.3. Significance of the Integrated Modeling Approach

In the very brief account above, we attempt to show a methodology to incorporate diverse categories of field-observed data into one single modeling analysis, in order to simulate unsaturated zone percolation patterns at Yucca Mountain.

Spatial heterogeneity clearly plays an important role in the pattern of percolation flux. So into this three-dimensional unsaturated zone model were incorporated, first, the large-scale heterogeneity data of tilted tuff layers and near vertical faults; second, the small-scale heterogeneity in measured matrix properties and derived fracture properties; and third the spatially distributed surface net infiltration for the upper model boundary.

The iterative forward and inverse numerical simulations were involved in the steps of calibration, first in 1-D using data in different boreholes, and then in 3-D to provide internal cross-check and validation for model prediction. The different categories of data play complementary roles in verifying different process and model conceptualization. For example, temperature data are useful to constrain percolation rates in the unsaturated zone; so also are the geochemical isotopic data that are sensitive to percolation. The significance of this integrated approach is that the problem at hand can only be solved by numerical modeling, yet it must be the measurements that can provide confidence to the model results. The integrated approach intrinsically integrates all possible data into the modeling: for input, for calibration, and for validation.

3.7. Concluding Remarks to Hydrological Issues in the Unsaturated Zone

The unsaturated zone in Yucca Mountain is complex. It is heterogeneous with alternating layers of non-welded to welded tuff with vastly different hydrological properties. There are also faults intersecting the layers that can provide fast episodic flow. The welded tuffs are characterized by relatively low matrix porosity and very low matrix permeability, yet intensely fractured. Experience from soil physics about capillary equilibrium of soil pores may lead one to believe that under partially saturated conditions, fractures should be void of water, and flow occurs only in matrix. Indeed air injection tests in the welded tuff give rise to high permeability that confirms presence of air-filled fractures. Yet geochemical field data indicate that flow is predominantly in the fractures. Much research has since led to a deeper understanding of fracture-matrix interaction in unsaturated fractured rocks.

In order to understand infiltration and percolation in the deep unsaturated zone, a large amount of different types of data were collected, and many specially designed field tests of different scales have been carried out in the Exploratory Studies Facility, the underground access via an 8 km tunnel to the welded and non-welded tuff layers. In addition, a three-dimensional unsaturated zone model with realistic representation of the layers, faults, and slopes has been developed. This model integrates the different types of data, including the spatially distributed infiltration map, liquid saturation, water potential, perched water, gas pressure, temperature logs, and pore water geochemistry, using them to calibrate the rock and hydrological properties of the different tuff units. This integrative approach offers an opportunity to verify various conceptualizations of the different processes in this complex system, and to enhance confidence in the model predictions.

4. Hydrologic Issues Related to a Nuclear Waste Repository in Clay Formations

4.1. Background and Introduction to Clay Rock Issues

Clay formations are considered in a number of European countries to be well suited for hosting radioactive waste repositories, because of their very low hydraulic conductivity and potential for self-sealing (of openings or fractures in the formations). Clay minerals also provide good sorption capacity for the retardation of radionuclide transport. Extensive studies of geotechnical issues related to the isolation properties of clay were conducted in underground research laboratories in Boom Clay in Belgium, a softer material dominated by plastic deformation since 1984 [Bernier *et al.*, 2007], and in argillaceous clays in France and Switzerland since 1990 [Delay *et al.*, 2010; Bossart and Thury, 2008]. In the U.S., Hansen *et al.* [2010] presented a feasibility study which indicated that radioactive waste disposal in a clay formation is also a possible option in U.S. The report states that the most desirable clay-rich rock to construct the repository should be at a depth between 300 and 900 m, with a thickness more than 75 m, and relatively homogeneous in composition and low in seismicity.

The features, events, and processes associated with radioactive waste disposal in clays have been catalogued and evaluated [Mazurek *et al.*, 2003] under the auspices of the Nuclear Energy Agency. Here features refer to structural characteristics of the clay formation such as bedding planes, events refer to external conditions such as heating from radioactive waste, and processes refer to physical or chemical processes such as solute diffusion through saturated clays. Much progress in the study of clays has been made over the past years and reported in the proceedings of a series of major international clay meetings: in ANDRA [2002, 2005b, 2007, 2010, 2012], and most recently in ANDRA [2015].

In its undisturbed state, clay has a high porosity but very low permeability, on the order of 10^{-20} m² or lower, and so there is not much hydrological concern. Probably the only issue is that of diffusion of

Figure 8. Hydrologic issues in clay arising from coupled THM processes.

dissolved solutes and gases in the pore water, but the diffusion coefficients tend to be very low, because of the low pore connectivity and high tortuosity. For the problem of a radioactive waste repository in clay, hydrological (H) issues arise mainly due to disturbances caused by mechanical (M) effects during excavation and ventilation of repository opening, thermal (T) effects from the heat-releasing radioactive waste, and chemical (C) effects of corrosion of engineered materials and radiohydrolysis of surrounding water that produce gases within the repository. They are part of the THMC coupled processes in geological formations discussed by Tsang *et al.* [2012].

Figure 8 illustrates the couplings between THMC processes. Mechanical effects during tunnel or repository excavation occur with the creation of a free surface, i.e., zero normal stress at the tunnel wall. With the presence of the “regional” in situ stress field, the stresses would redistribute around the opening and the rock deforms especially near the opening, resulting in what is called the excavation damaged zone (EDZ) around the tunnel [Tsang *et al.*, 2005]. Within this damaged zone, dependent on rock stiffness and cohesion and other mechanical property parameters, cracks or fractures may be formed that allow fluid flow through the clay rock. In time, however, the soft clay rock will settle and fractures will be self-sealed. The time required for self-sealing can be months or years. Also, as the tunnels are kept open over a period of decades to receive the waste into the repository for storage, air enters into the tunnel with relative humidity much less than 1. This causes drying of the clay rock near the tunnel surface, thus changing its mechanical property from that of ductile soft material to brittle. This, in turn, will result in changes in the fracture pattern within the EDZ. These processes are indicated in the right-hand side of Figure 8.

Since the radioactive waste releases heat, it is expected that there will be a temperature increase on the order of 100°C near the repository, depending on waste-emplacement density and local rock properties. The temperature would cause thermal expansion and other changes in mechanical properties of the clay rock, as well as impose thermal stresses in the rock. This is illustrated on the left part of Figure 8. Indicated on the lower left part of Figure 8 are the chemical processes of gas production through corrosion of waste canisters and engineered material in the repository and through radiolysis of surrounding water, which may give rise to gas accumulation and gas pressure in the repository.

The center column of Figure 8 shows three main hydrological issues for a waste repository in clay due to TMC-induced effects. The first is pore pressure changes, which are not due to an imposed or natural pressure gradient in the general flow field, but to a change in the local pore size, because of mechanical deformation or differential thermal expansion among water, clay skeleton, and solid. In high-permeability media, such pore pressure changes will dissipate quickly. However, for low-permeability clay rock, dissipation of the pressure change may take days, months, or even years. The second main issue is related to fluid flow in EDZ in clay. This includes thermally induced two-phase flow, changes in air relative humidity with desaturation (drying) and the related suction effect that affects the rock mechanical properties. Note that clay thermal conductivity is a function of water saturation and thus may be varying in space and time, and may well be anisotropic. Fluid flow is mainly through fractures in the EDZ, which undergo self-sealing over time, as

Table 1. Summary of Rock Properties and In Situ Conditions of Four URLs Located in Clays

Location	Mol (Belgium)	Mont Terri (Switzerland)	Bure (France)	Tournemire (France)
Rock formation	Boom Clay	Opalinus Clay	Callovo-Oxfordian argillite	Toarcian argillite
Age	Rupelian 30 Ma	Aalenian 170 Ma	Callovo-Oxfordian 155 Ma	Upper Toarcian 185 Ma
Water content (wt %, loss at 105°C)	22–27	6.6	7	3–4
Porosity (%)	39	16	18	7–8
Clay content (wt %)	23–59	66	55	55
Isotropic hydraulic conductivity (m^2)	2.4×10^{-19}	2×10^{-20}	5×10^{-21} to 5×10^{-20}	10^{-22} to 10^{-21}
UCS normal to bedding (MPa)	2	15	21 ± 6.8	32
Overburden in the rock lab (m)	233	250–320	495	250

part of the mechanical behavior of clay. The development of hydraulic conductivity over a long time period is an important issue.

The third main issue concerns the gases produced from chemical corrosion of engineered materials in the waste repository and from radiolysis of surrounding water. When the gas accumulates and its pressure exceeds the pore entry pressure, the gas begins to migrate through the porous clay rock, or if the pressure increase is fast and high, it may cause fracturing and thus form new flow paths for focused gas migration.

A review of recent studies on these three main hydrologic issues will be presented in the sections 4.3–4.5.

It may be noted here that the development and implementation of a clay repository are at an earlier stage than those in crystalline fractured rock and in unsaturated tuff formation. In the clay case, a repository license application has not yet been submitted to the regulatory authorities, and very intensive research on these coupled processes is ongoing through modeling, laboratory investigations, and particularly through field tests in underground research laboratories (URLs).

In the next subsection, four major URLs in clay formations that have been in operation over the last three decades are introduced and described. This is followed by three subsections summarizing recent studies related to the three main hydrologic issues described above. This section ends with a few concluding remarks.

4.2. Four Major URLs for Clay Repository Research

In this section, four major underground research laboratories (URLs) that have been devoted to clay repository research are briefly introduced. Since many of the research results in this area have been gained through these URLs and their supporting laboratory and modeling activities, this brief introduction will facilitate references to these sites when discussing clay hydrologic issues in later subsections. Representative properties of the rocks and conditions in the URLs are summarized in Table 1. The property values of these sites can be very different from each other, because of their different sedimentology history giving rise to different clay types and contents, and different ages with different tectonic history giving rise to different chemical consolidation and mechanical compaction.

The first URL shown in Table 1 is the High Activity Disposal Experimental Site (HADES) facility excavated at 223 m depth in Boom Clay, a tertiary clay formation in Mol, Belgium. Since its construction in 1980, many experimental investigations have been conducted at the site. Figure 9 shows the construction history of the HADES facility. The main tunnel is about 200 m in length, with an internal diameter averaging about 4 m, from which experiments were conducted in boreholes and side galleries. An extensive summary is provided by *Bernier et al.* [2007].

The second major URL is the French facility in Bure, at the border between Meuse and Haute-Marne, about 300 km east of Paris. Its construction started in 2000, with a target horizon for the URL between 420 and 550 m deep in argillaceous rock. The first experimental facility was completed in 2005 [ANDRA, 2005a]. Key details regarding the work on the Bure URL can be found in *Delay et al.* [2010], *Armand et al.* [2013, 2014], and *Willeveau et al.* [2006].

Figure 9. Layout of the HADES facility in URL at Mol, Belgium [Bernier et al., 2007].

The third major URL is the Mont Terri Facility in northwest Switzerland, located in an argillaceous formation known as Opalinus Clay. This is a generic research facility not located at a potential future repository site. Construction of the facility in conjunction with a motorway tunnel started in 1987, and research activities of the Mont Terri project were initiated in 1996 with multiple phases. The current phase is Phase VI, which was defined in 2003 with a 10 year planning horizon, but has been extended to 2018 with an expanded scope [Vomvoris et al., 2015; Bossart and Thury, 2008]. This is shown in Figure 10, which also serves to illustrate the extent of a typical URL and the successive stages of activities conducted in such a facility.

The fourth URL is the Tournemire Site in the south of France, which is also a generic research facility not located at a future repository site. This URL geological setting is characterized by a 250 m thick subhorizontal indurated argillaceous layer. A railway tunnel, constructed in 1881 through the argillaceous formation, is 1.8 km long, 6 m high and 4.7 m wide, and was excavated using a pneumatic tool. In 1996, two 30 m long, 3.7 m high, and 4 m wide horizontal tunnels were excavated off the main railway tunnel. Then, in 2003, another 40 m long horizontal tunnel was excavated. Thus, this facility enables study of near-field rock behavior in indurated clay, including the impact of water desaturation, over different time periods of exposure to the atmosphere, namely 129, 14, and 7 years, respectively [Millard et al., 2009; Massmann et al., 2009]. In 2008, this URL was extended with the excavation of two additional galleries to conduct a new series of experiments [Barnichon et al., 2011].

Figure 10. The layout of the Mt. Terri Laboratory (2015). From Mont Terri Consortium, Swisstopo [Vomvoris et al., 2015].

Figure 11. Pore pressure evolution in the three packed intervals in boreholes HG-A2 and HG-A3. The top three curves correspond to data from HG-A3. From Mont Terri Consortium, Swisstopo: *Marschall et al.* [2006].

4.3. Pore Pressure Changes

In general, excavation induces a multiphysics coupled response in the rock around the tunnel. Rock movements resulting from excavation induce a volumetric deformation of the pore space which, when coupled with the low rock hydraulic conductivity, gives rise to strong pore water pressure variations that will then dissipate slowly. These pore pressure changes have a significant influence on the effective stress state in the rock and may contribute to failure processes. Such pressure changes have been measured many tunnel diameters away from the tunnel wall, and these changes can last for months.

Marschall et al. [2006] reported a field study of pore pressure changes due to tunnel excavation in indurated clay. A horizontal microtunnel (13 m long and 1 m diameter) was drilled in an overconsolidated claystone (Opalinus Clay) formation in the Mont Terri URL within the Jura Mountains, Switzerland. The indurated clay has low permeability ($\sim 2 \times 10^{-20} \text{ m}^2$), a self-sealing capacity, low rock strength, and anisotropic geomechanical properties, with much of its properties sensitive to water content and saturation. It is highly fractured, but the fractures are generally tight at the in-depth stress conditions.

Before excavation of the microtunnel, 12 boreholes (HG-A2 to HG-A13) were emplaced and instrumented. In two of the boreholes, HG-A2 and HG-A3, hydraulic triple packer systems were emplaced for pore pressure measurements. The triple packer system separates each of the boreholes into three monitoring intervals, labeled “i1,” “i2,” and “i3,” corresponding to, respectively, 14–12.5, 12–9.5, and 9–5.5 m along the borehole.

Figure 11 shows the pore pressure evolution in the monitoring intervals in HG-A2 and HG-A3 during tunnel excavation (at the rate of 1.5 m/h). Pore pressure changes in HG-A2 (lower three curves in Figure 11) are significantly smaller than those in HG-A3 and exhibit some anomalous behavior. This behavior can be explained by HG-A2 being significantly farther from the tunnel than HG-A3, and experiencing a higher “destress” because of the excavation directly below it. Further, a hydraulic communication between monitoring intervals A2-i1 and A2-i2 was detected immediately after packer inflation. For these reasons, only the pore pressure evolution in BHG-A3 (upper three curves in Figure 11) should be considered.

Before excavation, pore pressure in HG-A3 ranged between 0.75 and 0.9 MPa. Immediately after excavation was initiated, a significant rise was seen in all three monitoring intervals. The stepwise drilling procedure used was reflected in the pore pressure increases during this time. After termination of tunnel excavation, pore pressure continued to increase to a peak of 2.1, 1.9, and 1.75 MPa in intervals A3-i3, A3-i2, and A3-i1, respectively. Three weeks after excavation ended, pressures started to decrease steadily. The continuing later steady decrease of pore pressure may not be related to the microtunnel, but to the growing cone of depression due to pore water drainage into a nearby gallery.

The pore pressure increase during excavation can be explained by rock compression under undrained conditions, resulting from the immediate reaction on the stress redistribution, as with plastic clay or crystalline rock, while the continued increase for 3 weeks after termination of excavation may result from progressive

failure processes in the tunnel near-field and a time-dependent growth of the EDZ, leading to continuous redistribution of stresses until a semistable equilibrium is reached. Monitoring of deformations and pore pressures in all 12 observation boreholes suggested a quasi-continuous evolution of the damaged zone around Gallery 2004 and the microtunnel, including strength degradation of the rock because of the varying ventilation conditions. Tunnel ventilation created extended desaturation joints when the humidity inside the tunnel was low and caused rock softening when the humidity was high.

The experiment was simulated by a number of modeling studies [Levasseur, 2010]. For example, Arnedo *et al.* [2012] used an anisotropic hydromechanical constitutive model to explain the observed different responses in pore water evolution, depending on the orientation of the observation points with respect to bedding direction and the tunnel axis.

Similar observations on pore pressure changes during tunnel excavation have been reported at the Tournemire URL during excavation of the 2003 gallery [Massmann *et al.*, 2009], and at the Bure URL in the REP and SUG mine-by-tests [Wileveau and Bernier, 2008]. Sharp changes in pore pressure were also observed in the Boom Clay following excavation. In that case, dilation caused by unloading (decreased volumetric stress) led to suction and negative pore pressure that could not be recorded by piezometer filters. Then, at some point, cracks formed and the measured pressure increased abruptly from 0 to atmospheric pressures [Bernier *et al.*, 2007; Bastiaens *et al.*, 2006].

4.4. Fluid Flow

4.4.1. Excavation Damaged Zone and Coupled THM Processes

The construction of an underground tunnel in a clay formation represents a major perturbation, with new hydromechanical boundary conditions on the rock at the tunnel walls. The stress field is redistributed around the tunnel, and the tunnel surface is free to move inward until restrained by tunnel lining and support. Creating the underground opening also influences the rock mass properties. The region adjacent to the tunnel rock may change from water-saturated to unsaturated conditions (or at least suction can develop), which can change rock behavior from plastic to brittle [Delage *et al.*, 2007]. A suction increase may result in a pseudocohesion effect that may enhance rock strength. All these changes may result in the creation of an EDZ around the tunnel, the properties of which may vary over time [Tsang *et al.*, 2005; Davies and Bernier, 2005].

This damaged zone represents a region of enhanced permeability with porosity increase or the creation of tensile or shear fractures [Bossart *et al.*, 2004; Mertens *et al.*, 2004; Blümling *et al.*, 2007; Marschall *et al.*, 2006; Corkum and Martin, 2007]. An initial increase in permeability of 5 orders of magnitude has been measured at Mont Terri [Bossart *et al.*, 2002]. A similar magnitude increase was measured at Bure URLs (4–5 orders) [see Armand *et al.*, 2013] and at Tournemire (5–6 orders around the 1996 and 2003 galleries) [see Matray *et al.*, 2007], whereas at Mol, a 2 orders of magnitude increase was observed by the time the first measurements were made. However, this effect decreases over time because of clay swelling and clay creep behavior, especially in cases where swelling refill materials are used to provide a back pressure on the rock [SELFAC, 2007; Lanyon *et al.*, 2009; Volckaert *et al.*, 2004].

As an example, Figure 12 shows EDZ patterns around a tunnel in plastic clay at Mol in Belgium. A herringbone structure of fractures was found around the tunnel, extending 1 m in the radial direction and 6 m axially forward of the tunnel front face. The fracture spacing was about 0.5 m. Similar patterns are also found in stiff clay at Bure, France [Armand *et al.*, 2013, 2014; Wileveau and Bernier, 2008]. Some theoretical and numerical models have been developed in an attempt to simulate such a pattern and the processes leading to it [Van den Eijnden *et al.*, 2015; Pardoën *et al.*, 2015; Yao *et al.*, 2015].

The EDZ extent and intensity do not depend simply on whether the clay is plastic or stiff (as at Mol or at Bure, respectively), but on other rock properties, including variability and heterogeneity, the anisotropy of the stress field, the overconsolidation ratio, and the presence of bedding planes [Escarffier *et al.*, 2005; Popp and Salzer, 2007; Popp *et al.*, 2008; Gens *et al.*, 2007].

Tunnel ventilation and temperature changes may have a strong influence on rock properties [Gerard *et al.*, 2008], since they may cause desaturation in the near field. Desaturation, in turn, gives rise to capillary forces and hence an increase in rock cohesion and strengthening, while at the same time it increases tensile stress and the potential for bond failure, and furthermore may also change the degree of property anisotropy.

Figure 12. Fracturing pattern around a gallery in Mol: (left) cross section perpendicular with gallery axis; and (middle) vertical cross section parallel to gallery axis, and also around (top right) a resin-immobilized borehole and of (bottom right) a retrieved core. (Adapted from *Bernier et al.* [2007].)

All these cause changes in the EDZ, with its system of large fractures (herringbone type) and smaller fractures, which form the pathways for fluid flow.

4.4.2. Fracture Resealing in the EDZ

As mentioned earlier, the fractures may close and seal due to clay deformation and moisture-induced swelling. This is an important process, because it results in a decrease in EDZ permeability. A number of studies have been conducted to investigate swelling behavior and permeability evolution [*SEFRAC*, 2007; *Lanyon et al.*, 2009; *Zhang and Rothfuchs*, 2008].

Creep occurs especially in plastic clay, but it can also occur in indurated clay, possibly leading to long-term tunnel convergence for unsupported tunnel walls and to an increase in the EDZ extent. A number of studies have been conducted to investigate sealing of fractures [e.g., *Naumann et al.*, 2007; *Labrousse et al.*, 2009]. Figure 13 shows results from a set of laboratory experiments on fractured Opalinus Clay samples from Mont Terri conducted under confined conditions. After deliberate fracturing, creep-induced fracture closure is shown as a slow reduction of hydraulic conductivity over a period of 200 days.

Decay heat from radioactive waste has to dissipate away through the buffer and the near-field rock to the far field. (Although initially before repository closure, the heat release through the open ventilated drifts will be significant.) At the same time, clay resaturation occurs and it is a slow process governed by low rock permeability and buffer characteristics, and will not be uniform over the repository domain. Heating will lead to steam convection in the inner region of the desaturated repository near field. Further, heating will generate transient pore pressure buildup resulting from differential thermal expansion, leading to changes in effective stress state. Heating may also affect some other relevant processes discussed in the previous section, such as possibly changing creep rate and strength. Studies addressing heating effects using laboratory measurements and field tests include those by *Collin et al.* [2002], *Gens et al.* [2007], *Sultan et al.* [2002], *Tang et al.* [2008], *Cui et al.* [2009], and *Sillen et al.* [2010]. Two major URL experiments to study these THM processes will be described in a later section.

4.4.3. Modeling of Coupled THM Processes in Clay

The complex-coupled THM processes in clay formations have been considered theoretically and incorporated into numerical models, so that the processes can be understood quantitatively. Based on a discussion of factors

Figure 13. Evolution of hydraulic conductivity with time in fractured Opalinus Clay samples under confined conditions [*Labrousse et al.*, 2009].

associated with these coupled processes by *Gens et al.* [2002], Table 2 was developed to illustrate the elements needed for developing coupled THM models.

As a side note to this table, the validity of Darcy's Law to describe advective flow in clays has been studied and modifications of Darcy's Law have been suggested especially for unsaturated clays [see e.g., *Liu and Birkholzer*, 2012].

Based on the elements presented in Table 2, the numerical simulation model CODE_BRIGHT was developed [*Olivella et al.*, 1996; *UPC*, 2014] which has been widely applied to clay THM problems. This code has also been

Table 2. Variables and Equations for Modeling Coupled THM Processes

Variable	Equation	Remarks
Liquid and gas advective flows	Darcy's law	Function of porosity, saturation, and temperature (via viscosity)
Vapor diffusion	Fick's law	Includes also tortuosity from clay porous medium
Thermal conduction	Fourier's law	Depends on ϕ and S ; specific heat of materials is additive
Liquid phase saturation	Retention curve	Accounts for suction or capillary pressure; includes hysteresis
Liquid and gas densities; solid density (expansion)	Density equations	Function of temperature and pressure
Phase viscosity	Liquid and gas viscosity equations	Function of temperature
Stress tensor	Mechanical constitutive model	Includes explicitly effects of strain, suction, and temperature
Dissolved air mass fraction	Henry's law	Including effects of temperature and capillary pressure
Vapor mass fraction (vapor pressure)	Psychrometric law	

applied to the modeling of gas flow through unsaturated clay rock by implementing gas migration in association with the development of preferential flow paths through pressure-dependent fractures in clay [Olivella and Alonso, 2008].

A number of other THM simulators have also been developed. One example is the TOUGH-FLAC code, which combines the well-established multiphase, multicomponent flow code TOUGH2 with the commercial-standard soil and rock mechanics code FLAC3D and the BBM geomechanical representation of clay behavior [Rutqvist *et al.*, 2002, 2011, 2014]. Another example is the OGS code [Kolditz *et al.*, 2012], which provides a finite element model framework in which multiphase flow and thermomechanical processes have been implemented and tested against laboratory data [Wang *et al.*, 2014]. These are powerful tools that can be used to simulate and understand THM processes in clay formations.

4.4.4. Major THM Experiments

A large number of field experiments on various aspects of THM behavior in clay have been carried out in the underground research laboratories (URLs) described in section 4.2. Summaries of the activities may be found in ANDRA [2015, 2012], which also serve as good resources for further references.

Figure 14. The HE-E experiment layout at Mont Terri URL [Vomvoris *et al.*, 2015] behavior of the clay and bentonite buffer system as both the near-field rock and the bentonite buffer are gradually saturated with water. Construction of the experiment took place from December 2010 to June 2011. Heaters were then turned on in July 2011, and the bentonite-heater interface reached 140°C in 1 year, after which the temperature was kept constant.

In this section, we present two examples of major experiments in the URLs to illustrate the sophistication and detailed consideration that have entered into such experiments.

The first is the so-called HE-E experiment [Gaus *et al.*, 2012; Vomvoris *et al.*, 2015], which is being conducted in the Mont Terri URL. It is a heater experiment in the Opalinus Clay formation involving two heaters of 30 cm diameter emplaced in a 50 m long tunnel of 1.3 m diameter. The heaters are surrounded by a bentonite buffer at very low initial water content and emplaced in two separate sections of the tunnel (Figure 14). The bentonite is also a clay material with a large capacity of swelling as its water content or saturation increases. The aim of the experiment is to investigate thermally induced THM processes.

Figure 15. The PRACLAY in situ experiment comprises the Gallery & Crossing Test, the Seal Test and the Heater Test [Van Marcke *et al.*, 2015].

The buffer between the heater and the Opalinus Clay rock experienced a very strong temperature gradient, because of the low thermal conductivity of the unsaturated bentonite buffer. While the temperature at the heater-buffer interface is 140°C, the temperature at the outer buffer-rock interface is around 40°C 18 months after start of heating. With heating, the vapor is driven out from the heaters, and there is an increase in relative humidity farther out at the buffer-rock interface, probably because of condensation with lower temperatures at the larger radius. Natural water inflow from the Opalinus Clay toward the buffer occurs slowly through diffusion. Both the relative humidity and liquid pore pressure have been measured at monitoring points at different distances from the heating source. An initial effort in modeling of the relative humidity and the pore pressure behavior by Garitte *et al.* [2015] gives moderately satisfactory results.

The second URL experiment to be described here is the PRACLAY heater test that is being conducted in plastic Boom Clay at HADES URL in Belgium [Van Marcke *et al.*, 2015; Li *et al.*, 2015]. The PRACLAY Gallery is 45 m long with a diameter of 2.5 m. It was excavated perpendicularly out from an existing gallery called the Connecting Gallery (Figure 15). Heaters are emplaced in the deeper 30 m section of the PRACLAY Gallery, and water-saturated sand is emplaced within the gallery around the heaters to provide quasi-undrained boundary conditions. The goal of the experiment is to understand the hydromechanical processes induced by excavation and then the thermo-hydro-mechanical processes induced by the heater test. Extensive monitoring of the clay behavior has been set up in boreholes from the gallery itself and from the neighboring Connecting Gallery.

The heaters were turned on in October 2014 to heat the gallery up to 80°C at the gallery walls, and then the temperature will be maintained at that level for at least 10 years. Predictive THM modeling has been conducted in 3-D to predict the Boom Clay behavior during heating [Chen *et al.*, 2015]. Model results show that the pore pressure will increase significantly at the beginning of the heating phase, because of the different thermal expansion coefficients of water and the clay skeleton. The maximum pore pressure could reach up to 3 MPa after 1.5 year heating, and then the overpressure will dissipate gradually through the low-permeability Boom Clay. The EDZ around the gallery created during excavation will be extended slightly during the heating phase, due to the weakening of the clay by the increase in temperature. These and other prediction results will be tested against field data in the coming months.

Compared to the HE-E experiment in the Mont Terri URL, the PRACLAY Heater test is being conducted in much softer plastic clay (Boom Clay) instead of the undurated clay (Opalinus Clay). Also, the hydraulic boundary condition at the gallery wall (being in contact with water-saturated sand) is very different from that at the HE-E tunnel wall, which is initially in contact with the bentonite buffer at low water content. A comparative study of the results from these two tests, and an understanding of their similarities and differences, will help to advance our knowledge of THM processes in clay formations.

4.5. Gas Migration Through Clays

Gas production from corrosion and degradation of repository engineering materials, and the related pressure buildup and transport, are also outstanding issues that have received considerable attention [see e.g., Marschall *et al.*, 2005; Olivella and Alonso, 2008]. If the gas production rate is large compared with the rate of diffusion of dissolved gases in pore water, then the solubility limit will eventually be exceeded, and discrete gas phase will be formed within the clay formation. The gas pressure will then build up until it exceeds the gas entry pressure of the clay pores, and it will enter into the clay medium and move along preferred paths

Figure 16. Layout of the HG-A gas-leak-off test at the Mont Terri URL (test section at front end of tunnel, magapacker position in green and backfilled section in red). From *Marschall et al.* [2008].

of least resistance. Alternatively, if the gas pressure buildup is fast and high, it may induce mechanical effects in the clay formation and create fractures or enlarge the size of EDZ.

Of particular interest is the international cooperative project named FORGE, which involved 24 organizations in 12 European countries [Shaw, 2015]. It was designed to address key research issues related to the generation and movement of repository gases, by means of a series of laboratory and field experiments. These were accompanied by comprehensive modeling activities.

The FORGE project was strongly linked to in situ experiments, among which are the PGZ1 experiment at Bure URL and the HG-A experiment at Mont Terri URL. The PGZ1 experiment at the Bure URL is dedicated to observing the different gas transfer mechanisms: advection-diffusion of dissolved gas, two-phase flow, dilatancy-controlled flow, and flow in macroscopic tensile fractures [de La Vaissière and Talandier, 2015]. Several test phases are dedicated to characterizing a specific mechanism at a time.

The HG-A is a gas-leak-off test that studies the processes and parameters associated with the migration of gas generated in the repository along tunnels and into the host rock. The experiment consists of a dead-end microtunnel with a large packer that seals off a test region at the tunnel end (Figure 16). The tunnel, excavated in 2005, has a length of 13 m and a diameter of 1 m. Monitoring was conducted before, during, and after tunnel excavation. A series of water injection tests were then performed in 2007–2008 [Marschall et al., 2008]. After studying the self-sealing of the excavation damage zone in the region of the packer over some years, tests with gas injection into the test interval were initiated in 2010. Along with many other parameters, the gas pressure built up in the test section has been monitored. A semianalytical model has been developed to understand these data [Alcoverro et al., 2014]. The key aspect included in the model analysis is the investigation of fracture opening and closure in the EDZ in response to water and gas injections. Under a number of simplifying assumptions, a relatively simple model was developed that can nevertheless reproduce the main trends of the observed pressure evolution in the test section of the HG-A experiment.

The FORGE project has concluded with the results published in 2015 as a Special Publication 415 of the Geological Society of London. A good summary of the results may be found in Shaw [2015] and Norris [2014].

In one particular study within the FORGE project, Zhang [2015] conducted a series of laboratory tests on clay cores, as well as field experiments, in order to study gas permeability changes in clay during the steps from undisturbed clay formation, to creation of an EDZ during repository construction at a depth of 400–800 m, and finally to the step when the fractures in the EDZ are resealed and gas is restricted behind the confining clay rock. He suggested the following evolution in permeability related to gas leakage through

clay: (a) gas permeability in undisturbed clay is negligible; (b) with excavation damage, gas permeability can increase by several orders of magnitude up to a level of 10^{-16} to 10^{-21} m², assuming a confining stress of 10–20 MPa; (c) as water enters and flows through fractures, the clay matrix takes up water and expands into the interstices, so that the water conductivity decreases dramatically down to 10^{-19} and 10^{-21} m² within short periods of months to years, even at a low confining stresses of 2–4 MPa; and (d) the gas in the clay would then rise in pressure; and it is found that at a gas pressure of 8–11 MPa, it is able to overcome the gas entry pressure of resealed fractures in clay at a depth of 500 m, and thus gas is able to leak through the resealed fractures without fracturing the clay formation. This finding by Zhang [2015], if confirmed, implies the existence of certain characteristics in the pore structure of resealed fractures, which allows gas leakage but not water flow. This deserves further studies.

4.6. Concluding Remarks on Hydrologic Issues in Clay

The hydrologic issues related to clay formations mainly relate to coupled thermo-hydro-mechanical THM processes, as shown in Figure 8. This includes pore water pressure changes due to stress-induced deformation of the pores, or differential thermal expansion of water and pore skeleton. Fluid flow in clay is possible through fractures in the EDZ. The flow rates and flow patterns are very dynamic in nature, subject to changes resulting from dehydration and hydration of the clay in the vicinity of the fractures, as well as any temperature gradient imposed. Flow may eventually be stopped when the fractures in clay are resaturated with water and become sealed because of clay swelling. Finally, gas flow through clay under various mechanical and thermal conditions has also been studied in depth.

While much work has been done over the last 30 years through field tests, laboratory investigations, and model simulations, there is still much room for further studies of the complex-coupled THMC processes, especially in the temporal development of hydrologic processes in clay. Future studies, though focused on hydrology, would require some significant knowledge of rock mechanics, thermal transfer, and chemical interaction. This makes this line of research both challenging and interesting.

5. General Concluding Remarks

The sustained interest in the performance assessment of radioactive waste repositories in various geological formations over the last 35 years has provided an opportunity for significant advances in certain aspects of the hydrologic sciences, especially those related to flow and transport. In this paper, we reviewed the hydrologic issues related to three major geologic formations being considered as possible hosts to waste repositories—namely, crystalline fractured rock, unsaturated zone volcanic tuff, and plastic or undurated clays.

For each of these rock types, we have chosen to emphasize a different hydrologic aspect. For crystalline rock, the focus is on flow and transport in saturated fractured rock from a repository depth of about 500 m to the shallow subsurface. For the unsaturated zone, the focus is on flow through the unsaturated zone from the shallow subsurface to the repository depth, also through a fracture-matrix rock system. For clays, since the permeability is very low, the focus is on hydrologic issues that arise because of mechanical and thermal perturbations in clay, which are referred to as coupled thermo-hydro-mechanical processes.

The studies for all three rock types are subject to demands not usually encountered in other applications of hydrogeology, such as a prediction period of hundreds of thousands of years with a spatial scale of several kilometers, and the need to account for early arrival of relatively small amounts of flow and contaminants, rather than the mean arrival time. For these reasons, studies of these hydrologic issues have been quite intensive, focusing on slow as well as fast processes. They include not only detailed modeling studies and comprehensive laboratory tests, but also large-scale, multiyear field experiments. All these have produced a very valuable data and knowledge base, which should be of interest to the general hydrologic community.

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