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Abstract

This review describes the state-of-the-art in hydrogeological modelling for safety-case studies related to spent-fuel repositories in crystalline hard rock, focusing on issues of relevance for the KBS-3 disposal concept in Nordic environments. The review includes a survey of model capabilities and assumptions regarding groundwater flow processes, geological and excavation-related features, and boundary conditions for temperate, periglacial, and glacial climates. Modelling approaches are compared for research sites including the Stripa mine (Sweden), the Grimsel Test Site (Switzerland), the Whiteshell Underground Research Laboratory (Canada), the Äspö Hard Rock Laboratory and Simpevarp-Laxemar site (Sweden), the Forsmark site (Sweden), the Waste Isolation Pilot Plant site (USA), and Olkiluoto (Finland).

Current hydrogeological models allow realistic representations, but are limited by availability of data to constrain their properties. Examples of calibrations of stochastic representations of heterogeneity are still scarce. Integrated models that couple flow and non-reactive transport are now well established, particularly those based on continuum representations. Models that include reactive transport are still mainly in the realm of research tools.

Thus far, no single software tool allows fully coupled treatment of all relevant thermal, hydraulic, mechanical, and chemical transport processes in the bedrock, together with climate-related physical processes at the ground surface, and with explicit treatment of bedrock heterogeneity. Hence practical applications require combinations of models based on different simplifications.

Key improvements can be expected in treatment of the unsaturated zone, simulation of heterogeneous infiltration at the surface, and hydromechanical coupling. Significant advances have already been made in the amounts and types of data that can be used in site-scale models, including large datasets to define topography and other surface conditions. Current tools also allow comparisons in terms of time-dependent flow and hydrogeochemistry, for the purpose of model calibration and confirmation.

The growth in model complexity has led to increased realism, but at a cost of increased computational demands which can limit possibilities to explore uncertainty. Future technological improvements may depend on proprietary tools that raise obstacles for regulatory review. An additional risk is that particular models may be developed to such a level of sophistication that viable alternative models might be discounted, due to lack of comparable resources.

Important weaknesses in the state-of-the-art include the limited understanding – both in terms of concepts and data – for periglacial and glacial environments, which must be considered for assessment periods on the order of 100,000 years.

GEIER Joel (Clearwater Hardrock Consulting). Paikkamittakaavan kovan kallion hydrogeologian mallinnusmahdollisuuksien vertailu turvallisuusarviointitarkoituksiin. STUK-TR 15. Helsinki 2012. 54 s.

Avainsanat: hydrogeologia, kiteinen rakoillut kallio, hydrogeologinen mallinnus, radioaktiivinen jäte, KBS-3-konsepti

Tiivistelmä

Raportointi esittelee huipputason mallinnusmenetelmiä, joita voidaan hyödyntää kovaan kallioon suunniteltavien käytetyn ydinpolttoaineen loppusijoituslaitosten turvallisuusperusteluissa. Työssä tarkastellaan pohjoismaisen KBS-3-konseptin kannalta relevantteja oletuksia, joita tehdään virtauksen kuvauksissa geologisissa muodostumissa, louhinnan aiheuttamissa rikkonaisuuksissa sekä niissä alku- ja reunaehdoissa, joita tehdään lauhkeille, periglasiaalisille ja glasiaalisille ilmasto-oloille. Vertailua tehdään esittelemällä mallinnuksia tutkimuspaikoilta, joita ovat: Stripa (Ruotsi), Grimsel (Sveitsi), Whiteshell (Kanada), Äspö ja Simpevarp-Laxemar (Ruotsi), Forsmark (Ruotsi), WIPP (USA) ja Olkiluoto (Suomi).

Hydrogeologiset nykymallit pystyvät todenkaltaisiin kuvauksiin, mutta niiden tarvitsemien ominaisuuksien määrittelyä rajoittavat puutteet käytettävissä olevissa mittausaineistoissa. Esimerkit heterogeenisuuden kalibroiduista stokastisista kuvauksista ovat edelleen harvassa. Virtauksen ja konservatiivisen kulkeutumisen yhteen kytkevät mallit ovat nykyisellään vakiintuneita. Mallit, jotka sisältävät reaktiivista kulkeutumismallinnusta ovat edelleen pääasiassa tutkittavan työkalun roolissa.

Toistaiseksi mikään yksittäinen ohjelmistotyökalu ei pysty kaikkien termisten, hydraulisten, mekaanisten ja kemiallisten kulkeutumisprosessien täysin kytkettyyn kuvaukseen kallioperässä, johon kytkeytyy myös ilmastomuutokset maanpinnalla ja myös kallioperän heterogeenisuuden kuvaus. Tästä syystä käytännön sovellutukset ovat yhdistelmiä malleista, jotka sisältävät erilaisia yksinkertaistuksia.

Mallinnuksiin ilmaantunee parannuksia saturoitumattomien vyöhykkeiden käsittelyssä ja hydromekaanisissa kytkennöissä. Paikkamalleihin voi jo nykyisellään sisällyttää aineistoja, kuten alueen topografia- ja muita pintaolosuhdetietoja. Nykyiset työkalut mahdollistavat myös ajasta riippuvat vertailut virtauksen ja hydrogeokemian välillä.

Lisääntyvä monimutkaisuus on johtanut mallien kasvavaan todenkaltaisuuteen. Samalla laskentavaatimukset ovat kasvaneet, joka voi rajoittaa epävarmuuksien tutkimusta. Tuleva kehitys voi tapahtua myös yrityssalaisuuksien piirissä olevilla työkaluilla, jotka voivat vaikeuttaa viranomaistarkastuksia. Riskinä voi olla myös, että yksittäinen mallinnusmenetelmä kehittyy niin korkealle tasolle, että ehkä taloudellisista syistä vähemmän kehitettyihin vaihtoehtoisiin mallinnustapoihin aletaan suhtautua varauksellisesti.

Huipputason mallinnusten keskeisiä heikkouksia – sekä konseptuaalisesti että tietoaineistojen suhteen – ovat periglasiaali- ja glasiaaliolojen ymmärrys. Turvallisuusperustelussa näitä on tarkasteltava satojen tuhansien vuosien mittakaavassa.

Contents

1 Introduction

1.1 Background

This review is intended to produce background information for STUK's safety appraisal work, to help STUK to prepare for issues that may arise in evaluation of a construction license application for a high-level radioactive waste repository.

In 2001 Finland's government granted a favorable Decision in Principle on Posiva Oy's application to locate a repository at Olkiluoto. According to Posiva (2008), Posiva aims to submit an application for a construction license for the disposal facility by the end of 2012. Since autumn of 2004, construction has been in progress for the ONKALO underground rock characterization facility, which will serve as part of the access to the planned repository, if the construction license application is approved.

1.2 Purpose and objectives

The purpose of this review is to describe the state-of-the-art on how hydrogeological modelling methods are utilized in safety-case studies for spent-fuel repositories in crystalline hard rock. Particular attention is given to:

- types of initial and boundary conditions,
- model calibrations, and
- uncertainty considerations

The focus is on issues of relevance for evaluating the robustness of the KBS-3 disposal concept, focusing primarily on issues that are of concern for Nordic coastal and near-coastal environments over the course of a glaciation cycle. Special emphasis is given to the level of quantification that is needed in models in order to indicate a sufficient level of confidence for safety assessment.

The review includes an assessment of the achievable levels of practical and/or reliable hydrogeological models that can be expected within the next 5–10 years (recognizing the high uncertainty regarding potential advances in computing technology over that time scale).

Models that have been developed for crystalline hard rock sites as part of high-level waste disposal research programmes in Sweden, Switzerland, France, and Canada are considered as examples for comparison. The emphasis of comparisons is on the available data, methodologies and successfulness, rather than on hydrological differences between the sites.

Along with a discussion of the leading edge in hydrological modelling and "best available technologies" for modelling, the requirements of Finnish legislation will be taken into consideration, specifically, the question of adequacy: when have the proponents demonstrated "well enough" that groundwater flow is sufficiently low in the repository near-field?

2 Survey of model capabilities and assumptions

2.1 Representations of groundwater flow processes

2.1.1 Saturated flow

Saturated flow of groundwater is represented in some form by all models that have been applied to site-scale simulations of hydrogeology in crystalline hard-rock environments. Two major types of representations are used: continuum and discrete-fracture representations. Hybrids of these approaches, including dual-porosity/dual-permeability models and numerically coupled continuum-discrete fracture models, have also been used.

Continuum representations

In porous-medium (continuum) models, flux of a single-phase fluid through the pore space is assumed to be related to hydraulic potential gradients according to Darcy's law:

$$\boldsymbol{q} = -\frac{1}{\mu_f}\mathbf{k}\left(\nabla p - \rho_f \boldsymbol{g}\right) \tag{1}$$

where $\boldsymbol{q} = \phi \boldsymbol{u}$ is the Darcy flux (or specific discharge), ϕ is the accessible (flow) porosity, $\boldsymbol{u}$ is the mean fluid velocity (vector), $\mathbf{k}$ is the permeability tensor, μ_f is the dynamic viscosity of the fluid, p is pressure, ρ_f is fluid density, and $\boldsymbol{g}$ is the gravitational acceleration vector with components $\{0, 0, -g\}$ in a given $\{x,y,z\}$ coordinate system with z vertically upward.

As discussed in a later section of this report, a continuum representation may not necessarily be valid for models of fractured, crystalline hard rock. The key question is whether Darcy's law is actually valid for the fractured rock on scales of relevance; in other words, whether a permeability tensor $\mathbf{k}$ can actually be defined for a given block scale in the model, such that the foregoing equation holds for all directions of the hydraulic potential gradient. Efforts to confirm this assumption by upscaling from discrete representations (for example, Long et al., 1982 and Khaleel, 1989) have produced mixed results depending on scale and connectivity of the fracture system.

However, despite these questions about the applicability of Darcy's law, continuum representations are still often used in modelling of repositories, particularly for the larger scales of consideration, and for considering complex processes that are more difficult to evaluate with discrete models. With these caveats, the following development proceeds from this central assumption.

Conservation of mass in the pore-fluid phase requires that divergence of the mass flux be balanced by the time rate of change in fluid mass that is stored per unit volume of rock:

$$\nabla \cdot (\rho_f \boldsymbol{q}) + \frac{\partial(\rho_f \phi)}{\partial t} = 0 \tag{2}$$

For a system in which porosity is influenced both by pore fluid pressure and by overburden stress σ, this can be expanded as:

$$\nabla \cdot (\rho_f \boldsymbol{q}) + \frac{\partial(\rho_f \phi)}{\partial p}\frac{\partial p}{\partial t} + \frac{\partial(\rho_f \phi)}{\partial \sigma}\frac{\partial \sigma}{\partial t} = 0 \tag{3}$$

or:

$$\nabla \cdot (\rho_f \boldsymbol{q}) + \frac{S_s}{g}\frac{\partial p}{\partial t} - C\frac{\partial \sigma}{\partial t} = 0 \tag{4}$$

where S_s is specific storage, representing the increase in water that can be stored per unit pore volume, per unit increase in pressure (due to the combined effects of water compression and pore volume expansion), and C is a poroelastic coefficient describing the change in pore volume per unit increase in overburden stress.

For the commonly considered situation where the fluid is water at constant density ρ_w and viscosity μ_w, Darcy's law can be expressed more simply as:

$$\boldsymbol{q} = -\mathbf{K}\nabla h \tag{5}$$

where **K** is the hydraulic conductivity tensor which is related to the permeability tensor as:

$$\mathbf{K} = \frac{\rho_w g}{\mu_w}\mathbf{k} \tag{6}$$

and h is hydraulic head:

$$h = \frac{p}{\rho_w g} + z \tag{7}$$

In combination with conservation of fluid mass, this leads to the flow equation:

$$\nabla \cdot (\mathbf{K}\nabla h) = \frac{S_s}{\rho_w g}\frac{\partial p}{\partial t} - \frac{C}{\rho_w}\frac{\partial \sigma}{\partial t} \tag{8}$$

For a given point in crystalline hard rock, changes in the elevation component z of hydraulic head over time are ordinarily considered to be negligible in comparison with changes in the pressure component $p / \rho_w g$, i.e.:

$$\frac{\partial h}{\partial t} \approx \frac{1}{\rho_w g}\frac{\partial p}{\partial t} \tag{9}$$

For short time scales (less than a year) such as those considered in models of hydraulic testing, this approximation is generally valid. Changes in overburden stress can also usually be neglected on short to intermediate time scales, yielding the simplified flow equation:

$$\nabla \cdot (\mathbf{K}\nabla h) = S_s\frac{\partial h}{\partial t} \tag{10}$$

For long-term modelling of groundwater evolution in a Fennoscandian setting, these simplifications in the flow equation (negligible changes in elevation and confining stress) might not hold. Bedrock elevation changes gradually relative to sea level, due to glacial loading and post-glacial unloading effects (isostatic rebound). In longer-term situations (for example, modelling of a complete glaciation-deglaciation cycle), the groundwater pressure changes associated with glacial loading and unloading are generally large compared with the changes in bedrock surface elevations. However, the time scales for glacial loading and retreat can differ from that for isostatic compensation in the Earth's mantle.

For two-dimensional flow (for example in tabular fracture zones or other tabular aquifers, treated as porous continua), the corresponding simplified flow equation is:

$$\nabla \cdot (\mathbf{T}\nabla h) = S\frac{\partial h}{\partial t} \tag{11}$$

where **T** is the transmissivity tensor in the plane of the aquifer, and S is storativity. In the case of non-horizontal aquifers, the gradient operator is taken with respect to a 2-D coordinate system aligned with the plane of the aquifer.

Groundwater models that have been used for repository applications generally assume that the hydraulic properties (**K** and S_s or **T** and S) are homogeneous at least on the scale of the discretization that is used (a mesh element in a finite-element model, or a grid cell in a finite-difference model).

In addition, many models assume that the hydraulic properties are isotropic ($\mathbf{K} = K\mathbf{I}$ or $\mathbf{T} = T\mathbf{I}$, or where **I** is the identity matrix and K and T are scalar values of hydraulic conductivity and transmissivity, respectively).

With these assumptions of local homogeneous and isotropic properties, the 3-D and 2-D flow equations simplify further to:

$$\nabla^2 h = \frac{S_s}{K}\frac{\partial h}{\partial t} \tag{12}$$

and:

$$\nabla^2 h = \frac{S}{T}\frac{\partial h}{\partial t} \tag{13}$$

For steady-state flow, or for quasi-steady flow over long enough time scales that changes in fluid storage can be neglected, the change in head with time is effectively zero, so the flow equation simplifies to:

$$\nabla^2 h = 0 \tag{14}$$

for both the 3-D and 2-D cases.

Dual-porosity/dual-permeability formulations

More complicated types of continuum representations have been developed for fractured, porous rock in which the fracture system is assumed to be ubiquitously connected, so it is represented as a continuum which is coupled to porous-medium blocks which have porosities and/or permeabilities that contrast with the continuum that represents the fractures. Mathematically, these models consist of flow equations similar to the preceding equations for simple continuum models, but with a separate flow equation for each part of the system, and coupling terms that describe flow between fractures and matrix or vice versa.

Early instances of this type of model were developed primarily for fractured petroleum reservoirs (e.g. Warren and Root, 1963), but the concept has also been applied to water flow and solute transport in fractured crystalline rock. The main property that distinguishes between dual-porosity/dual-permeability models is that they are able to represent the different time scales of response, for flow and transport in response to changing boundary conditions. The concept has been extended to multi-porosity models to account for variable matrix-block sizes in fractured crystalline rock (Neretnieks and Rasmuson, 1984).

More geometrically complex representations of dual-permeability systems, in which the fractures form an irregular network, are discussed below in the context of DFN models.

Discrete-fracture network representations

Discrete-fracture network (DFN) models take into account the discontinuous and irregular connectivity of fracture networks. They are primarily useful for rock with relatively sparse fracture networks, such as is ordinarily sought for radioactive-waste repositories in crystalline hard rock.

DFN representations are generally based on three principles:

1) An equation that describes the relationship between flow and the gradient of hydraulic potential within the plane of a given, single fracture;
2) Continuity of hydraulic potential at each point along intersections between fractures; and
3) Conservation of mass (fluid flux) across fracture intersections.

The equation describing saturated flow within a given fracture is developed from either of two assumptions, which for practical purposes lead to equivalent mathematical representations.

The classical approach (Snow, 1969) is based on a parallel-plate conceptual model for flow through a single fracture. Assuming a fracture with uniform aperture b, and Newtonian fluid of uniform density ρ_f and viscosity μ_f, and flow that is laminar and quasi-steady or creeping (i.e., inertial forces due to fluid acceleration are negligible), fundamental considerations of fluid mechanics lead to the "cubic law" for flowrate density (flowrate per unit width of fracture):

$$\boldsymbol{q}_f = -\frac{\rho_f g b^3}{12\mu_f}\nabla h \tag{15}$$

where the gradient operator is with respect to a 2-D coordinate system within the plane of the fracture. Conservation of mass leads to a flow equation of the form:

$$\nabla \cdot \left(\frac{\rho_f g b^3}{12\mu_f}\nabla h\right) = S_f \frac{\partial h}{\partial t} \tag{16}$$

where S_f is an effective fracture storativity.

An alternative approach is to assume that each fracture can be described in terms of an equivalent, 2-D "aquifer" of finite extent, with effective hydraulic transmissivity T_f and S_f), with a flowrate density:

$$\boldsymbol{q}_f = -T_f \nabla h \tag{17}$$

This approach accommodates fractures for which the effective transmissivity is a lumped product of variable aperture, permeable fracture fillings, breccias etc. It can also accommodate fractures with anisotropic effective transmissivities:

$$\boldsymbol{q}_f = -\mathbf{T}_f \nabla h \tag{18}$$

where $\mathbf{T}_f$ is a 2-D tensor in the plane of the fracture. Conservation of mass leads to a flow equation:

$$\nabla \cdot (\mathbf{T}_f \nabla h) = S_f \frac{\partial h}{\partial t} \tag{19}$$

which is of identical mathematical form to the flow equation for 2-D flow in an aquifer.

In the case in which the fracture transmissivity is isotropic within each discrete fracture (i.e. $\mathbf{T}_f = T_f\,\mathbf{I}$, the only case that is ordinarily considered in saturated-flow models for repository applications) case, this simplifies to:

$$\nabla \cdot (T_f \nabla h) = S_f \frac{\partial h}{\partial t} \tag{20}$$

By defining a hydraulic aperture b_h such that:

$$b_h = \sqrt[3]{\frac{12\mu_f T_f}{\rho_f g}} \tag{21}$$

or:

$$T_f = \frac{\rho_f g {b_h}^3}{12\mu_f} \tag{22}$$

this flow equation may be written as:

$$\nabla \cdot \left(\frac{\rho_f g {b_h}^3}{12\mu_f} \nabla h \right) = S_f \frac{\partial h}{\partial t} \tag{23}$$

which is identical in form to the corresponding flow equation as derived from the cubic law. Thus, for both ideal and non-ideal fractures, a flow equation of the form:

$$\nabla \cdot (T_f \nabla h) = S_f \frac{\partial h}{\partial t} \tag{24}$$

can be used as the basis for discrete-fracture flow models.

In practice, estimates of transmissivity deduced from in-situ well testing are generally considered to be more reliable for predicting fracture flow properties, than estimates based on aperture measurements in combination with the cubic law (NRC, 1996, p. 344). Hence this is the approach usually taken, except in coupled hydromechanical models that account for changes in aperture as a function of rock stresses and fluid pressures (as discussed in Section 2.1.4).

Combined DFN/porous-medium representations

A few models have been developed which allow 3-D simulation of flow through irregular fracture networks with coupled porous-medium matrix blocks.

The MAFIC code (Miller et al., 1995) uses an explicit discretization of a DFN model and treats the adjoining matrix blocks as a coupled porous continuum, with each block being represented by an idealized geometry (spheres, cylinders, or slabs). Transient flow into and out of a given matrix blocks can occur only via the nearest flowing fracture. Thus this representation does not account for the possibility of large-scale flow via the matrix; through-flow takes place only via the fractures.

The FRAC3DVS model (Therrien and Sudicky, 1996; Therrien et al., 2003) simulates flow and transport in planar fractures which are represented as 2-D planar features, and matrix blocks which are modeled in 3-D. Curviplanar fractures are mapped onto the orthogonal faces of brick-shaped elements so that computations can be made on an orthogonal grid.

The FEFTRA model (Löfman et al., 2007) allows explicit simulations of dual-permeability systems with arbitrarily complex fracture geometries. This is done by an octree algorithm for generating a fully 3-D finite-element mesh of the fractures and surrounding space, in which the matrix is discretized as 3-D elements, while fractures are represented by 2-D elements along the faces of the 3-D elements that abut the fractures. In typical workstation configurations, applications of FEFTRA have considered relatively simple fracture geometries, e.g. just the main deformation zones at the Olkiluoto site (Löfman and Mészáros, 2005). The model has been applied for simulations of a DFN model for a full repository layout, apparently using a supercomputer, but some calculation cases were found to be computationally intractable due to high numbers of solution nodes (Hartley et al., 2010).

2.1.2 Unsaturated flow

Unsaturated flow occurs in the phreatic zone in the upper bedrock and overburden. In the porous continuum case, parameterization of this requires a more complicated form of the flow equations in which the fluid storage term (specific storage, in 3-D) is replaced by terms that represent partial saturation of the pore space, and permeability or hydraulic conductivity becomes a function of moisture content (or alternatively, pressure/suction). This leads to a flow equation of the form (Evans et al., 2001):

$$-\nabla \cdot \boldsymbol{q} = \nabla \cdot \left[\mathbf{K}(\theta) \nabla h \right] = \frac{\partial \theta}{\partial t} \tag{25}$$

where $\boldsymbol{q}$ is the volumetric flux vector and $\mathbf{K}(\theta)$ is the hydraulic conductivity as a function of volumetric water content. $\mathbf{K}(\theta)$ is typically a nonlinear function of the porous medium. This type of equation can be solved with finite-difference techniques, but generally requires iterative solution techniques which are demanding in terms of computational resources. As noted by Evans et al. (2001), there is no proven method for measuring $\mathbf{K}(\theta)$ in situ, due in part to the complication that the water in partially saturated media is under negative pressure heads and cannot be extracted from the rock without applying a more strongly negative pressure by means of a porous plate, membrane, or similar arrangement.

Hydrogeological models that account for unsaturated-zone flow in a porous continuum include the

MIKE SHE modelling tool (DHI Software, 2009), which has been used for modelling near-surface flow in the Swedish repository programme (Bosson et al., 2010). In the work described by Bosson et al. (2010, p. 59), the number of grid cells for the unsaturated zone is limited by an algorithm in order to reduce the complexity of computations.

Unsaturated flow in discrete-fracture networks

Discrete-fracture network models that account for fluid flow through variably saturated fractures were presented by Rasmussen (1988; 1991) and by Kwicklis and Healy (1993). Results showed that partial saturation within fractures can result in increased fluid velocities and faster solute transport. However, measuring the properties of discrete fractures that govern unsaturated flow in situ poses difficulties at least as difficult as those for porous media.

The Yucca Mountain repository project in Nevada, USA, resulted in extensive development of conceptual models for groundwater flow through fractured porous rock, due to the importance of unsaturated-zone processes for the repository concept. As described by Pruess (1999; 2001), laboratory experiments and numerical simulations of fluid mechanical processes at a fundamental level (capillary effects, imbibition on porous fracture surfaces, film flow over rough fracture surfaces, etc.) were used to simulate processes that contribute to areally distributed seepage in fracture networks. Faybishenko et al. (2001) describe similar conceptual-model developments for vadose-zone flow in fractured basalts in the Snake River Plain in southeastern Idaho, US, based on field experiments, physical laboratory models (textured glass plates), and numerical simulations using the TOUGH2 code (Pruess, 1991).

In most circumstances of interest for deep repositories in hard crystalline rock in Nordic settings, the unsaturated zone is thin (on the order of a few meters) and is usually neglected for the sale of simplicity in simulations of the deep hydrogeological system. Exceptions may include modelling of drawdown during the operational phase of a repository. However, even then the details of partial saturated-unsaturated flow are commonly neglected.

Models such as DarcyTools (Svensson et al., 2004) and FEFTRA (Löfman and Mészáros, 2005) instead use an adjustable-free-surface approach to account for desaturation of the upper bedrock. The position of the interface is calculated by an iterative method: Grid cells with negative pressures in the first iteration are considered to be above the free surface and are excluded from the next iteration. Grid cells containing the interface are assigned a reduced effective hydraulic conductivity based on the thickness of the saturated portion of the cell. Pressures are recalculated, the free surface is again adjusted, and so on until a stable result is obtained.

Painter and Sun (2005) modelled the drawdown due to a repository used an explicit two-phase (gas, liquid), two-component (air, water) model in a continuum model with homogeneous properties. They conclude that an adjustable free-surface approach (neglecting unsaturated zone processes) gives adequate predictions of steady-state flows and maximum inflows. However, they also find that the free-surface approach could lead to overestimation of transient inflows by as much as 70%, during the dewatering phase of repository construction and operation. This could be a concern, if observed inflows are used as part of the acceptance criterion for deposition holes.

2.1.3 Coupled density-dependent flow and diffusion of salinity

For models of coastal settings, or where brines are found at depth, the water density can vary as a function of salinity variation within the region being modeled, and flow is driven by the interaction of density and pressure gradients. Thus the effects of salinity gradients on groundwater flow need to be considered. At the same time, salinity gradients give rise to diffusion which acts to reduce the salinity gradients, and groundwater flow also leads to hydrodynamic dispersion as fluids of contrasting density are carried along different paths through the porous medium.

In a porous medium, these coupled processes are described by coupled partial differential equations, including the foregoing equations for conservation of fluid (water) mass:

$$\nabla \cdot \left(\rho_f \boldsymbol{q}\right) + \frac{\partial\left(\rho_f \phi\right)}{\partial t} = 0 \tag{26}$$

(in which $\boldsymbol{q}$ is related to pressure and density gradients by Darcy's law), and an equation for each dissolved chemical species, describing advective-dispersive transport with coupled diffusion into/out of matrix blocks:

$$\begin{aligned}\frac{\partial\left(\phi\rho_f c_{fi}\right)}{\partial t} &+ \nabla\cdot\left(\rho_f \boldsymbol{q} c_{fi}\right)\\ = \nabla\cdot\left(\phi\rho_f \mathbf{D}\nabla c_{fi}\right) &- 2wD_e\left(\frac{\partial c_{mi}}{\partial w}\right)_{w=0}\\ \frac{\partial\left(\phi_m \rho_f c_{mi}\right)}{\partial t} &= D_e\frac{\partial^2 c_{mi}}{\partial w^2}\end{aligned} \qquad (27)$$

where c_{fi} and c_{mi} are the mass fractions of species i in the fractures and matrix blocks, respectively, $\mathbf{D}$ is the dispersion tensor, 2ω is the flow-wetted surface (interfacial area between flowing fractures and matrix) per unit volume of rock, ϕ_m is the matrix porosity, D_e is the effective diffusion coefficient for the rock matrix, and w is the distance into a matrix block from the nearest fracture.

Numerical models capable of accounting for these coupled processes of density-dependent flow and advective-dispersive transport with matrix diffusion in a porous continuum include SUTRA (Voss and Provost, 2002), DarcyTools (Svensson *et al.*, 2004), FEFTRA (Löfman *et al.*, 2007), and NAMMU, the equivalent-continuum porous medium (ECPM) component of CONNECTFLOW (Jackson *et al.*, 2000; Hoch and Jackson, 2004). Thermal effects are also treated as a coupled process by some of these models.

Numerical models that account for these coupled processes in a discrete-fracture network have not yet been demonstrated for repository-scale simulations. Site-scale applications of the CONNECTFLOW code have however made use of ECPM permeabilities and porosities derived by DFN simulations of uniform-density flow in smaller blocks, and then applied in site-scale, density-dependent continuum flow models (Follin et al., 2008; Joyce et al., 2010). In coupled DFN-ECPM simulations presented by Hartley et al. (2006b,c; Joyce et al., 2010), groundwater densities calculated by the ECPM approach were interpolated onto a DFN component which accounted for fluid density-gradient effects within the fractures.

2.1.4 Coupled hydromechanical and thermal processes

Coupled hydromechanical processes arise from the interaction of pore (or fracture) fluid pressure p with the rock stress σ (tensor), and the elastic or inelastic response of the rock to the effective stresses $\sigma' = \sigma - p\mathbf{I}$ that result.

Fractured crystalline hard rock is relatively sensitive to fluid pressure due to the high aspect ratio of fractures compared to typical rock pores, and the reduced possibility for anomalous fluid pressures to dissipate via the rock matrix. As indicated by the "cubic law" for flow through a single, parallel-plate fracture, fracture transmissivity scales with the cube of aperture:

$$T_f \propto b^3 \qquad (28)$$

The component of effective stress σ_n normal to (across) a fracture tends to have a decreasing effect on aperture, as the compressive stress increases and aperture decreases. As discussed by Witherspoon et al. (1980), this happens because, for rough fractures, the contact area between opposing fracture surfaces increases with σ_n, increasing the fracture stiffness.

An empirical model describing this behavior is the Barton-Bandis joint model (Bandis *et al.*, 1983), which relates hydraulic aperture b_h to mechanical aperture b_m in terms of the fracture joint roughness coefficient JRC$_o$ as:

$$b_m\,[\mu\mathrm{m}] = \sqrt{b_h\,[\mu\mathrm{m}]\cdot JRC_o^{2.5}} \qquad (29)$$

and considers that the joint normal stiffness:

$$\kappa_n = -\frac{d\sigma_n}{db_m} \qquad (30)$$

increases hyperbolically as a function of the stress:

$$\kappa_n = \kappa_{no}\left(1 - \frac{\sigma_n}{\delta_m \kappa_{no} + \sigma_n}\right)^{-2} \qquad (31)$$

This model is implemented in the 2-D Universal Distinct Element Code, UDEC (Itasca, 2002), which has been used by Min (2004) for modelling coupled mechanical and hydrologic response in network flow problems in fractured granitic rock. A three-dimensional version of the model, 3DEC (Itasca, 2003), is also available, but due to practical limitations on the number of fractures that can be modeled, site-scale applications have been limited to modelling of major deformation zones (e.g., Hakami and Min, 2009).

2.2 Representations of bedrock

2.2.1 Discrete fractures

In recent site-scale models for repository applications, discrete fractures are usually represented explicitly only in the portions of the model volume that are close to repository tunnels, boreholes, or other features where the discrete nature of flow is judged to be of critical importance. The remaining portions are generally modeled as an equivalent-continuum porous medium (*e.g.* Hartley *et al.*, 2006a; Follin, 2008), or as discrete representations at reduced resolution, lumping the contributions of smaller fractures into a grid of "equivalent discontinuum" features (Geier, 2008a). Both of these approaches have disadvantages; the former tends to "smear out" the discrete nature of flow and transport paths in the far field, while the latter might exaggerate the continuity of such paths.

An alternative upscaling method involving dual-permeability discrete representations was presented for 2-D networks by Clemo (1994). This method has the advantage of retaining the discrete nature of connectivity on multiple length scales while accounting for permeability due to smaller-scale fractures in a simplified way that permits larger-scale simulations. However, it has not been extended to practical applications in 3-D repository-scale models.

Within the portions of the models in which fractures are explicitly represented, the usual approach is to treat each individual fracture as having homogeneous hydraulic and transport properties (i.e., uniform transmissivity T_f and uniform transport aperture). Alternative formulations using variable-aperture fractures have been investigated using smaller-scale network models (Nordqvist et al., 1992; Painter, 2006). The latter study (Painter, 2006) concluded that aperture variation within fractures is of minor importance for large-scale transport, compared with contrasts between fractures. Tsang and Doughty (2003) have proposed a complex-fracture model to account for realistic fractures that may contain breccias, fault gouge, etc., and may also be multi-stranded; this model has been used for small-scale simulations on the scale of single-hole, injection-withdrawal tracer tests (Doughty and Tsang, 2009), but not for repository-scale modelling.

Channel-network representations have also been used to account for the observation that flow is often restricted to just a fraction of the fracture plane (Tsang and Tsang, 1987; Moreno and Neretnieks, 1993), or in order to simplify transport calculations (e.g. the JNC-Golder channel network model as described in Poteri et al., 2002). The channel network model of Moreno and Neretnieks (1993) has been applied as an alternative model for transport calculations in the Swedish repository programme.

Apart from these limited applications of channel-network models, discrete-fracture network (DFN) models are the primary method for representing fractures as discrete conductors in the bedrock. In DFN models, the fractures may be simulated as deterministic, stochastic, or conditionally stochastic features.

Deterministic representations are used when the location, extent, and orientation of particular fractures are well defined from data. This is sometimes possible for a few well-characterized fractures on the scale of in-situ experiments, such as the TRUE Block Scale experiments at the Äspö Hard Rock Laboratory in SE Sweden (Poteri et al., 2002). However, for site-scale models, only a small portion of the fractures (if any) can be characterized in this way.

Stochastic representations of fractures are most often based on statistical geometry rather than mechanical principles. The approach typically used in repository-related applications in the Fennoscandian Shield and similar environments is to describe fractures in terms of several (usually 3 to 5) fracture sets, each of which is characterized in terms of statistical models for the fractures' spatial, geometrical, and hydraulic properties. The fractures are represented either as elliptical/circular disks (Baecher et al., 1977; Dershowitz, 1984; Dverstorp and Andersson, 1989) or as rectangles (Robinson, 1984; Herbert et al., 1991) depending on the implementation. Cross-validation exercises performed as part of the International Stripa Project (Fairhurst et al., 1993) indicated that, when the fractures are approximately equidimensional, either type of representation can produce similar results, provided that the models are based on the same statistical definitions of the fracture sets. Black et al. (2007) showed that models with strongly non-equidimensional fractures can lead to fundamentally different results in terms of connectivity. Table 1 lists the types of statistical models that are most commonly employed for these attributes of fracture sets.

Table 1. Statistical models commonly used for stochastic fracture set attributes in DFN models for hydrogeological simulations. Detailed definitions for most of these models are given by Dershowitz *et al.* (1998); additional references cited within table refer to examples of applications.

Fracture property	Most common statistical model(s)	Other models that are sometimes considered
Location/intensity	Simple Poisson process with uniform fracture intensity in a given fracture domain	Lévy fractal process (Hermanson *et al.*, 2005); simple Poisson process with gamma-distributed intensity (Hermanson *et al.*, 2005; 2008); compound Poisson processes such as parent-daughter process (Billaux *et al.*, 1989), nearest-neighbor model (Geier *et al.*, 1990) or exponential halo model (Geier, 2011).
Orientation (pole direction or normal vector)	Fisher distribution	Bingham distribution; nonparametric bootstrap resampling of measured poles after correcting for sampling bias.
Shape	Equidimensional shapes (circles, squares, or other regular polygons approximating a circle)	Ellipses with aspect ratios of 1:5 to 1:10 (Black *et al.*, 2007) to mimic hypothetical sparse channel networks.
Size (length or radius)	Pareto (power-law) distribution	Lognormal or exponential distribution.
Transmissivity	Lognormal distribution	Correlation to fracture size (Hartley *et al.*, 2005; 2006a).
Hydraulic aperture	Proportional to cube root of transmissivity	Proportional to square root of transmissivity (Dershowitz *et al.*, 2003; Hartley *et al.*, 2006a)

Conditional stochastic DFN models are a special case of stochastic DFN models, in which observed portions of fractures are matched explicitly, while maintaining consistency with the fracture statistics. Conditional DFN simulations are useful for applications where results are sensitive to the precise locations of particular fractures that have been mapped. Examples include:

- simulating the hydraulic response and tracer recovery in hydrogeological tests that are focused on particular borehole-fracture intersections,
- simulating radionuclide release from tunnels that have been mapped prior to waste package emplacement, where deposition holes are located in order to avoid particular fractures;
- simulating large fractures (or minor deformation zones) that are of a scale approaching the depth of a repository in a site-scale model

Dverstorp and Andersson (1989) presented a methodology for conditional simulations of a DFN model to match fracture traces as mapped in tunnels. They applied this to the rock around the 3-D migration drift in the Stripa underground research facility in Sweden. Conditional simulation of fractures intersections with boreholes using the CONNECTFLOW code was used by Follin *et al.* (2008) to allow more realistic comparison between simulated and actual wellbore flow logging results. A generalized methodology for conditional simulation to match fracture traces on tunnel walls or outcrops, as well as fracture intersections with boreholes, has been implemented in the DFM code (Geier, 2010).

A unique type of conditional DFN model was applied in the Canadian repository programme (Srivistava, 2002). This model is quasi-mechanistic, based on a set of geostatistical rules to mimic the process of fracture propagation, rather than simply reproducing statistics for fracture size, orientation, and intensity. The simulations were conditioned on regional-scale lineaments maps, so that the simulated fractures accounted for these lineaments, but varied stochastically at depth.

2.2.2 Equivalent-continuum porous media

Equivalent porous-medium, or equivalent-continuum porous medium (ECPM) representations of the bedrock are normally used for the major part of site-scale or regional-scale models, in repository applications. These models are normally constructed as finite-element or finite-difference models with rectangular blocks (usually cubes), and are parameterized in terms of an equivalent, block-scale permeability tensor $\mathbf{k}_s(\boldsymbol{x})$ or hydraulic conductivity tensor $\mathbf{K}_s(\boldsymbol{x})$ for each block of length scale s, centered at a given point $\boldsymbol{x}$. For brevity in the discussion that follows, we will refer to the block-scale hydraulic conductivity tensor $\mathbf{K}_s$, with the understanding that conversion between $\mathbf{k}_s$ and $\mathbf{K}_s$ is straightforward.

The current scientific consensus is that $\mathbf{K}_s(\boldsymbol{x})$ for fractured crystalline hard rock is best derived from a statistical DFN model of the bedrock, although alternatives based on application of geostatistical spatial averaging theories to well test data have also been applied (e.g. Norman, 1992a). Several different approaches have been used to derive $\mathbf{K}_s(\boldsymbol{x})$ from DFN models, and to apply these values in ECPM models.

A method developed for calculating $\mathbf{K}_s(\boldsymbol{x})$ for 2-D cases by Long et al. (1982) involves "permeameter" simulations in multiple orthogonal directions for each block (Figure 1), followed by fitting of an ellipse, representing the tensor, to the calculated flows as a function of pressure/head gradients. Applicability of the tensor concept for a given block is evaluated based on the goodness-of-fit. The method has also been extended to 3-D cases (e.g. Geier and Axelsson, 1991; Hartley et al., 2005). However it is computationally intensive for 3-D blocks containing large numbers of fractures, due to the need to discretize the fractures into a computational mesh for each block orientation. This must be done for each block scale that is investigated.

Geier et al. (1992) developed an alternative method that allows simultaneous estimation of $\mathbf{K}_s(\boldsymbol{x})$ for multiple scales s and potentially multiple block locations $\boldsymbol{x}$ from a single computational mesh. This is done by applying head gradients in different

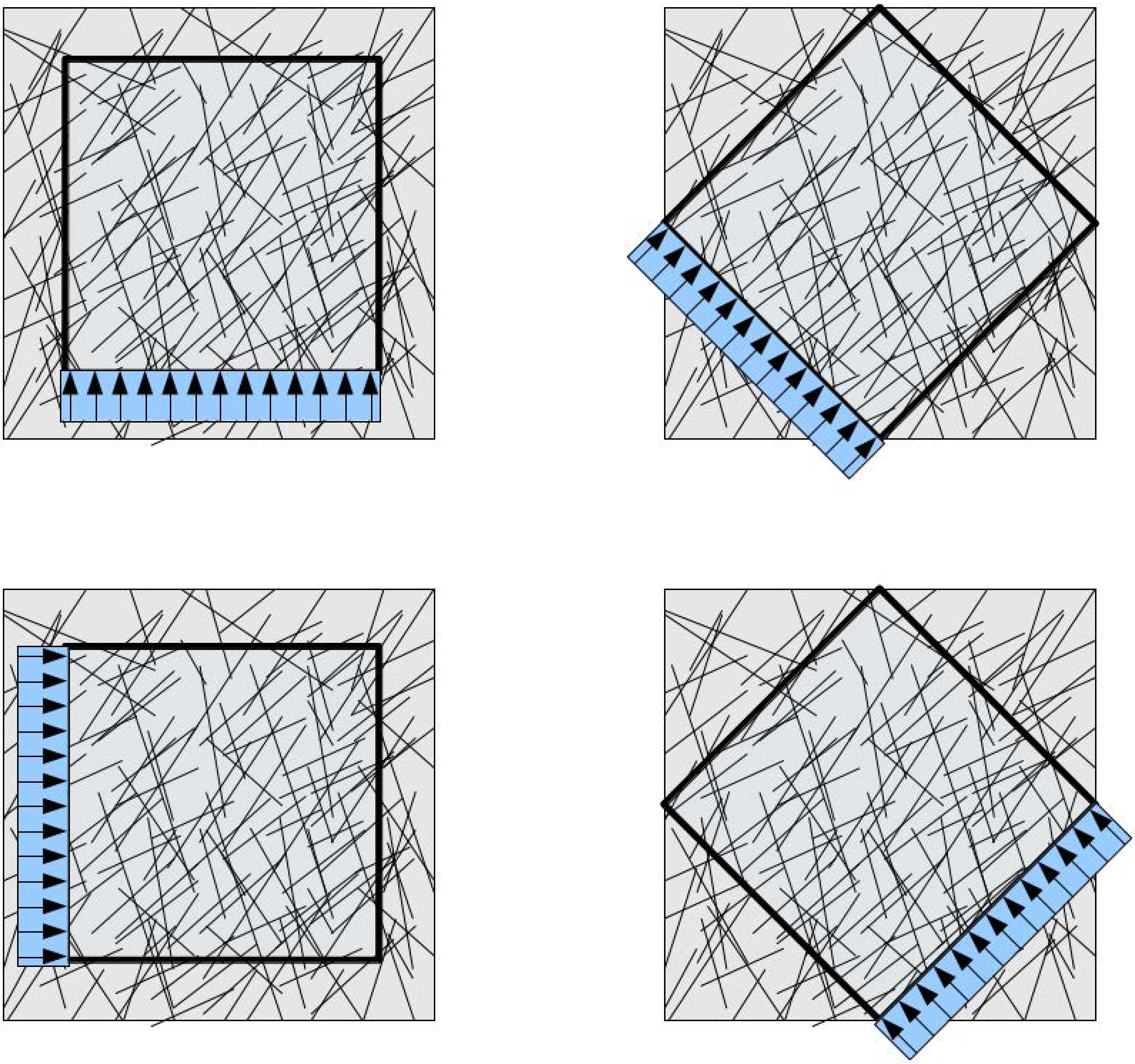

Figure 1. Block-scale permeameter simulations by imposing head gradients to a DFN realization in different orientations to determine effective directional permeabilities.

linear combinations, and then computing directed-surface integrals of flux and head gradients over different sub-volumes of the computational mesh. Goodness of fit and applicability of the tensor concept is assessed by an extension of the same approach as Long et al. (1982).

Applying this method in combination with a nested DFN simulation method (Figure 2), Geier et al. (1992) produced nonparametric estimates of covariance matrix functions, to describe the geostatistical variation, i.e. the covariance of the components of $\mathbf{K}_s(\boldsymbol{x}+\boldsymbol{h}) - \mathbf{K}_s(\boldsymbol{x})$ for a given separation vector $\boldsymbol{h}$ (also referred to as the "lag vector"). These functions can then be used as the basis for geostatistical simulations of ECPM models (e.g. Norman, 1992a,b). However, estimation of the geostatistical model is mathematically complex. Another drawback is that the ECPM models produced by this approach may not fully represent the spatial structure of $\mathbf{K}_s(\boldsymbol{x})$ that results from extensive, discrete structures. The difficulties increase when considering DFN models that are defined in terms of multiple fracture domains.

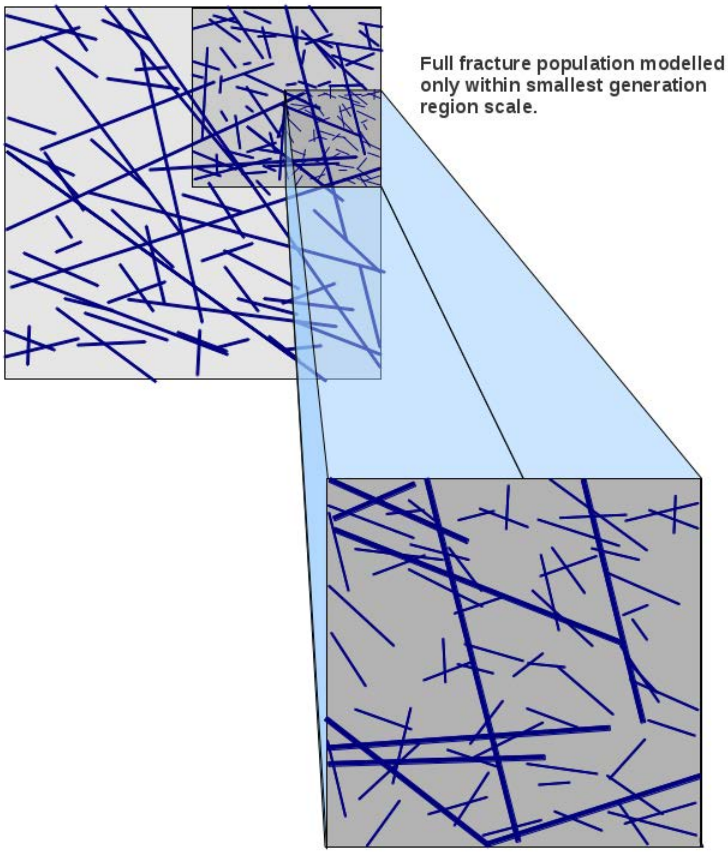

Figure 2. Nested generation method for producing block-scale simulations of a spatially heterogeneous DFN model for estimation of geostatistical properties, consistent with larger-scale simulations (after Geier *et al.*, 1992).

The CONNECTFLOW model (Hartley *et al.*, 2006a,b,c) takes a more direct approach to producing ECPM models based on DFN estimates of block-scale $\mathbf{K}_s(\boldsymbol{x})$. Conceptually, the discrete fractures for a given realization of the DFN model are simulated for the entire model volume, which is then divided into blocks so that the tensors $\mathbf{K}_s(\boldsymbol{x})$ for each block center $\boldsymbol{x}$ can then calculated by the permeameter approach of Long *et al.*, (1982). The values of $\mathbf{K}_s(\boldsymbol{x})$ are then assigned directly to the corresponding grid cell of the ECPM model. As a practical matter, the discrete fractures are not all generated simultaneously; fractures smaller than a given block scale are generated only as needed for permeameter simulations of each particular block, and then discarded after calculating $\mathbf{K}_s(\boldsymbol{x})$ for that block.

The main advantage of this direct approach used in CONNECTFLOW is that the spatial structure of the $\mathbf{K}_s(\boldsymbol{x})$ field is explicitly mapped onto the ECPM model, rather than through a process of geostatistical model fitting and then simulation, which can cause loss of details in this spatial structure. The approach can be applied to model volumes that contain multiple fracture domains, without the difficulties that arose in the approach of Geier et al. (1992) and Norman (1992). The main drawback is the amount of computations that are required to produce a site-scale ECPM based on a single realization of a DFN model, requiring access to a supercomputer for the largest models. This apparently was a consideration that limited the number of realizations of the DFN model that could be evaluated for SR-Site (SKB, 2011).

Another possible limitation of this approach is in the ability to treat DFN models that have more complex spatial relationships among fractures, rather than the simple Poisson (uniformly random) models for fracture location that have been analyzed in SDM-Site and SR-Site. For example, both weakly fractal DFN models and DFN models with fracture intensity that varies between blocks according to a gamma distribution were suggested as alternatives to the simple Poisson model for Forsmark (La Pointe et al., 2005), but these were not tested in the hydrogeological implementation of the DFN models.

A simpler, approximate method, as used in the DarcyTools model (Svensson et al., 2004) and as one option in the DFM model (Geier, 2008a, Marklund et al., 2008), is to estimate $\mathbf{K}_s(\boldsymbol{x})$ by summing the piecewise contributions of each fractures to the permeability tensor, based on each fracture's transmissivity and orientation, and the area of the portion of the fracture that is within the block. This uses the formula of Snow (1967) for the permeability tensor contribution that results from a set of fractures with uniform spacing and infinite extent, but with a geometrical scaling factor to account for the finite area of a fracture that is within a given grid block. As implemented in both DarcyTools and DFM models, the method is essentially the same as proposed by Oda (1985). The method generally overestimates the permeability of grid blocks, since it does not take into account the possibility that some fractures are not connected to a through-flowing network, or that part of each connected fracture's area could be in a "dead end" segment that does not contribute to flow.

None of these approaches directly addresses the question of how to handle blocks for which the fit to a tensor is poor. As shown by the results of Long et al. (1982), this assumption cannot be taken for granted in sparsely fractured rock. Geier et al. (1992) discuss error measures for the fitted permeability tensors, and their physical significance in terms of local flow magnitudes. However, a full analysis of the consequences for site-scale models incorporating such grid blocks has not yet been presented by any of the modelling groups that have presented ECPM models based on DFN model realizations.

2.2.3 Treatment of brittle deformation zones

Brittle deformation zones are recognized as broadly tabular (although possibly curved) zones within which fracture frequency is elevated in comparison with the surrounding bedrock. Geologically, these zones are usually interpreted as fault zones (whether active or, more often in shield settings, ancient but possibly showing evidence of episodic reactivation).

Site-scale models for repository purposes ordinarily treat brittle deformation zones as simple conductive surfaces which have either homogeneous hydraulic properties (Geier, 1996) or heterogeneous hydraulic properties which may be based on a geostatistical formulation (Geier, 1996) or simply random (Follin *et al.*, 2008). Results from Geier (1996) indicate that accounting for heterogeneity within these zones can significantly impact groundwater travel times for paths carrying radionuclides to the biosphere.

Geological investigations of fault zones (*e.g.* Caine *et al.*, 1996) reveal a complex architecture with fault cores (often with finely comminuted gouge and/or breccia) and associated damage zones. The detailed permeability structure of these zones is most likely not significant for predictions of site-scale flow, but may be significant for radionuclide transport. Secondary fracturing associated with the damage zone of fault zones can act as zones of reduced groundwater mobility that enhance retardation of radionuclides by diffusion in branching fractures, but act on different time scales compared with ordinary matrix diffusion, and can enhance long-term matrix diffusion (Geier, 2005).

Caine (1999) investigated the flow properties of four end-members for fault-zone structure, using explicit DFN models. Examples of site-scale flow models that incorporate this level of detail for brittle deformation zones are scant. One exception is a model of the Stripa Site Characterization and Validation Experiment (Dershowitz *et al.*, 1991) which treated the identified deformation zones as tabular zones of elevated fracture intensity, rather than as continuous features. However, this model did not represent the segregation between fault core or breccia zones and a less intensely fractured damage zone.

Accounting for the time-scale-dependent transport properties of these complex structures may require either multi-rate matrix diffusion models (Haggerty and Gorelick, 1995), or alternatively incorporating hydrogeological complexity that explicitly represents these variably mobile zones (*e.g.* Tsang and Doughty, 2003). The fraction of matrix diffusion capacity which is accessible over longer time scales via complex structures can be conservatively omitted in safety assessment models. However, when groundwater evolution (in terms of salinity or reference waters) modelling is used to calibrate or validate site-scale hydrogeological models, structural complexity associated with deformation zones might be important for matching time-scale dependent mass transfer.

2.3 Representations of other geological media and features

2.3.1 Unconsolidated sediments

Unconsolidated sediments (when present) form the surface of repository sites in crystalline bedrock. The technical term *regolith* has been used in the Swedish repository programme; this is defined as (Bates and Jackson, 1984):

> *The fragmental and unconsolidated rock material, whether residual or transported, that nearly everywhere forms the surface of the land and overlies the bedrock. It includes rock debris of all kinds – volcanic ash, glacial drift, alluvium, loess, vegetal accumulations, and soil.*

The regolith may be discontinuous, where bare outcrops of bedrock are exposed (although even such outcrops often have thin accretions of vegetative matter formed by lichens and moss, as well as surficial flaking and possibly products from chemical or biochemical microweathering processes, as described, e.g. by Nicholson, 2009). In the context of a Nordic repository setting where the bedrock is ancient, the regolith is also frequently referred to as "overburden" or "Quaternary deposits."

Major components of the regolith in coastal Nordic repository settings include glacial till, glaciofluvial sediments (including eskers), postglacial sands and gravels, clays, peat and gyttja (Johansson, 2008). Anthropogenic deposits (fill from modern construction projects, or disturbed ground from older excavations) may also be present. Typically all of these regolith units are discontinuous and of variable thickness, rather than forming continuous layers. Figure 3 illustrates a conceptual model of the regolith at the Forsmark site.

Data for the hydrological properties of regolith units may include slug tests, pumping tests, and BAT-filter tip permeability tests as well as laboratory permeameter tests (Johansson, 2008). Groundwater level monitoring data also can be used for model calibration and assessment of model accuracy.

In site-scale hydrogeological models, two different approaches have been taken. In models that focus on the deep bedrock, the regolith is often represented in a simplified way as a single layer with homogeneous properties. Models that focus on the interaction of surface waters and shallow groundwater (e.g. Bosson et al., 2008; 2010) may use a more detailed representation.

Models of bedrock hydrogeology for the Forsmark and Laxemar/Simpevarp areas (Hartley et al., 2006a,b,c) used a simplified regolith (till layer of uniform thickness) as a base case, but included a more complex, multi-layer representation of the regolith with lateral heterogeneity in subsequent cases.

Lake-bed deposits of low permeability (clays and gyttja) may impede vertical flow of groundwater. In a large-scale modelling study of the NE Uppland region that includes Forsmark, Holmén et al. (2003)

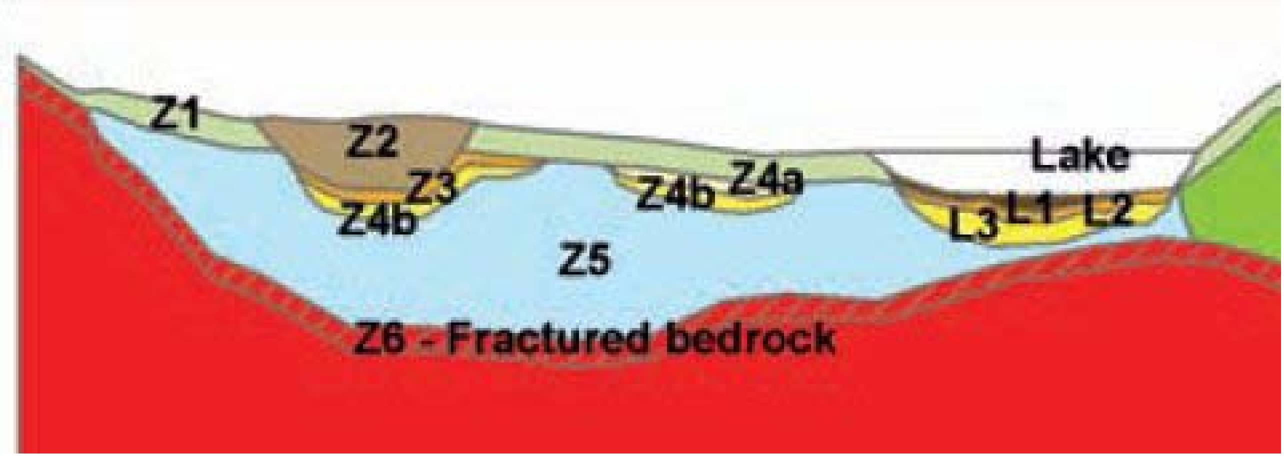

Figure 3. Conceptual model of regolith depth and stratigraphy. (Figure 3-2 from Johansson, 2008, SKB R-08-08, detailed discussion in Table 3-1 of Johansson, 2008). L1 = gyttja, gyttja/clay, and peat in lake beds; L2 = postglacial sand and gravel in lake beds; L3 = glacial/postglacial clay in lake beds; Z1 = surface layer affected by soil formation in terrestrial areas, or by sedimentation, transport and erosion in limnic/marine areas; Z2 = peat; Z3 = postglacial or glacial sand/gravel, fill; Z4a = postglacial clay including gyttja; Z4b = glacial clay; Z5 = till; Z6 = uppermost fractured bedrock.

applied a no-flow boundary condition to the base of lakes to represent the effect of an impermeable layer of clay/gyttja (but with specified heads equal to lakeshore elevation at the lake perimeters), but found that this had only a minor effect on regional recharge/discharge patterns. Observations of low groundwater heads below lakes, in relationship to the lake levels at Forsmark during dry summer periods (when evapotranspiration exceeds precipitation) and during pumping tests that produce local drawdowns of groundwater, indicate that seasonally downward flow from lakes to the bedrock is impeded (Johansson, 2008).

2.3.2 Excavation-damaged zone (EDZ)

The excavation-damaged zone (EDZ) is defined (Tsang and Bernier, 2005) as “a zone with hydrochemical and geochemical modifications, including significant changes in flow and transport properties.” Key aspects of relevance for site-scale hydrogeological models of a KBS-3 type repository, as illustrated in Figure 4, include additional fractures created by the excavation process (less so if full-face tunnel boring is used rather than drill-and-blast methods), plus the possibility of increased aperture on fractures that undergo shear displacement or stress relief depending on their orientation and position around the perimeter of the tunnel. Under conditions of high horizontal stress, spalling in the crown and floor of tunnels can also increase the hydraulic conductivity of the rock, in the direction along the axis of the tunnel.

A review of EDZ research conducted for SKB by Bäckblom (2009) concludes that the possibility of a continuous EDZ along deposition tunnels produced by the drill-and-blast method cannot be ruled out by data from experiments in Canada and Sweden, although the effects can perhaps be mitigated by careful control of the blasting method. The possibility to avoid development of axially extensive, blasting-induced fractures through carefully controlled drilling and blasting is supported by experiments at the Hard Rock Laboratory in Äspö, Sweden (Ericsson, 2009).

The hypothesis of a continuous EDZ along deposition tunnels has been simulated using discrete transmissive features in a rectangular, tube-shaped configuration along the tunnels (Geier, 1996; 2008a; 2011); the hydraulic conductivity of the backfilled tunnel is lumped into this representation. A similar approach but using just discrete two features in an inverted T-shaped configuration along each tunnel (one horizontal feature representing the EDZ along the floor of the tunnel, and one vertical feature running along the center plane of the tunnel) was employed by Hartley et al. (2006b,c) and Joyce et al. (2010), as shown in Figure 5. The advantage of the latter approach is to reduce the number of transmissive features that are needed to represent the tunnels, by a factor of two, while still providing an explicit pathway along the EDZ of the tunnel floor, which is likely to be the first part of the EDZ encountered by radionuclides leaking from a canister in the KBS-3V concept.

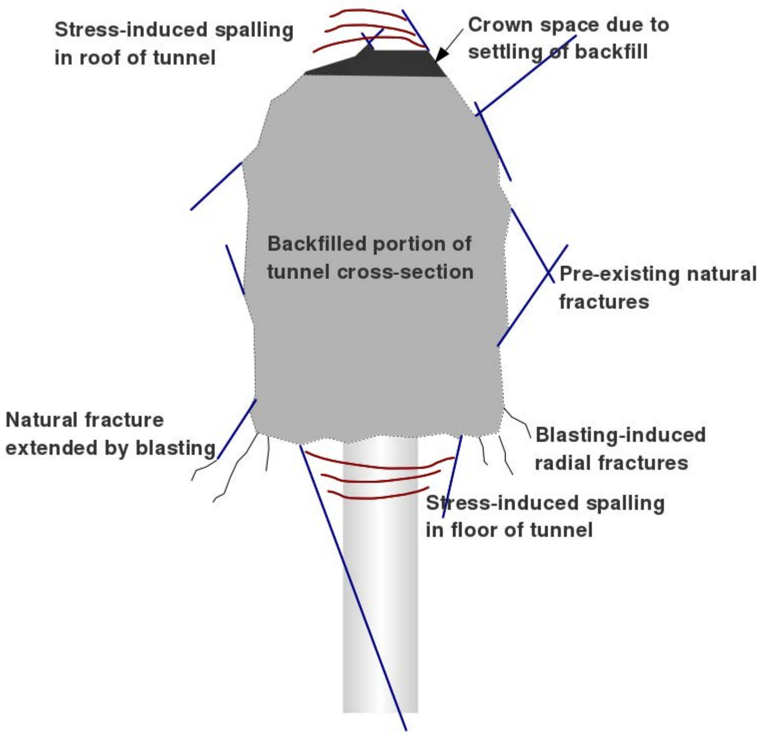

Figure 4. Schematic illustration of types of features that may contribute to hydrogeological properties of repository tunnels and the associated excavation-disturbed zone.

Svensson (2006) included repository tunnels and deposition holes in a model to estimate water inflows to a tunnel. The model is apparently for open-repository conditions; properties of the EDZ are not discussed.

Where repository tunnels pass through water-bearing deformation zones or high-transmissivity fractures, grouting may be specified to reduce inflows to the tunnels. Svensson (2006) accounted for grouting by modifying hydraulic conductivities within a 4 m thick layer around each tunnel. This is implemented as maximum-conductivity threshold: hydraulic conductivity is reduced to the specified target value K_{max} for grouting (two cases were considered, $K_{max} = 10^{-7}$ m/s and $K_{max} = 10^{-9}$ m/s). Effects of imperfect grouting (heterogeneous grout distribution) or excessive grouting were not considered in this approach.

An EDZ can also occur around deposition holes. Since the deposition holes are bored rather than blasted, the extent of this EDZ is normally expected to be just few millimeters into the rock. However, under conditions of high and anisotropic horizontal stress, stress-induced spalling could give rise to enhanced permeability along the sides of the deposition hole in the direction of the minimum horizontal stress. This situation has been evaluated with the discrete-feature modelling approach, by assigning increased permeabilities to two opposing sides of hexagonal prisms that are used to represent deposition holes (Geier, 2008a); results indicate that this could be significant for safety assessments.

2.3.3 Tunnel backfill and buffer

The KBS-3 concept calls for tunnels to be backfilled with bentonite or other clay-based materials that have low permeability and will swell as they saturate to fill any possible gaps. Hence the capacity of the backfilled tunnels to act as flow and transport paths should be minimal, and the surrounding EDZ should be more important.

Site-scale models that include tunnel layouts (e.g. Geier, 1996; Hartley et al., 2006b,c) have sometimes lumped the hydraulic conductivity and porosity of the backfilled tunnels with EDZ properties. In a smaller-scale model of the repository block for Laxemar, Hartley et al. (2006c) embedded a continuum porous-medium (CPM) model of repository tunnels and deposition holes, allowing a more explicit representation of the 3-D nature of flow through the backfill.

Backfilling experiments in the Canadian Underground Research Laboratory in Pinawa, Manitoba indicate a possibility for a gap to form in the crown space between the top of the backfill and the tunnel roof. The effect of a crown-space gap has been considered as a variant in recent simulations for Forsmark, using a continuum representation of tunnel backfill with a 0.1 m thick zone of increased hydraulic conductivity and porosity equal to unity at the top of the tunnels (Selroos and Follin, 2010).

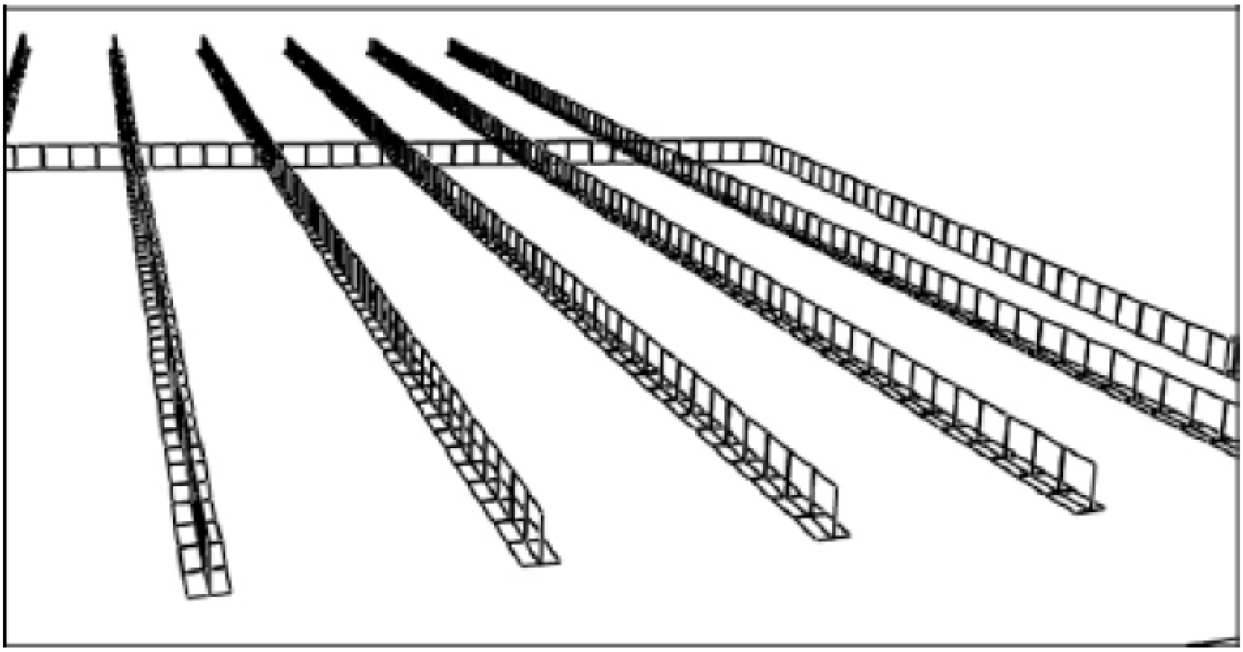

Figure 5. Discrete representation of repository tunnels and EDZ in floor of deposition tunnels, discretized into 7.5 m sections (from Hartley *et al.*, 2006b, SKB R-06-99).

The annulus of deposition holes should be filled with compressed bentonite blocks, which constitute the buffer. Buffer erosion was raised as a possibility in SKB's SR-Can safety assessment study (SKB, 2006), but thus far has not been addressed explicitly in site-scale hydrogeological models.

Details of flow and transport through the buffer are normally treated in near-field models on the scale of meters, while site-scale models are simply used to provide estimates of flows to deposition holes, which are used as input for the near-field models. However, these estimated flows may depend on the representation of the deposition holes and buffer in the site-scale flow model. Site-scale models that include deposition holes have generally treated these as if they were left unfilled (Geier, 1996; Svensson, 2006)

2.3.4 Unsealed boreholes

Boreholes used for site characterization could act as hydraulic connections through the bedrock, if left unsealed or imperfectly sealed. The KBS-3 repository concept calls for all boreholes to be sealed (SKB 2011), but conceivably some boreholes could be missed or seals could degrade. Unsealed boreholes may also need to be considered for models of the construction and operation phases of a repository.

One intuitive method for representing unsealed boreholes is to represent them explicitly with discrete conductors. However with this approach, the very high effective conductivity of an open borehole, compared with typical fractured bedrock, can lead to numerical difficulties in solving the flow equations.

An alternative method (Miller et al., 1995) is to represent boreholes by a net-flux boundary condition. This is a constraint that the sum of all inflows from fractures to a borehole, minus the sum of all outflows, should match the specified net flux (zero, in the case of a packed-off borehole which is otherwise left unsealed). The implementation by Miller et al. (1995) assumes that hydraulic head equilibrates instantaneously along the borehole (i.e., that the flow resistance of the borehole is effectively zero, compared with that of the fractures). This allows this condition to be implemented by row-and-column reduction in the matrix equations, leading to a reduction in the degrees of freedom of the equations. The method does not address situations where flow along the borehole could be driven partly by fluid density differences between fractures that intersect that borehole at different depths.

2.4 Representations of surface boundary conditions

Groundwater flow in the bedrock is ultimately driven by surface conditions. In temperate conditions such as prevail in coastal environments in Nordic countries, important processes at the site scale include precipitation (both rain and snow which may melt sometime after it falls), evapotranspiration (direct evaporation and transpiration by plants), diurnal or storm-related fluctuations in sea

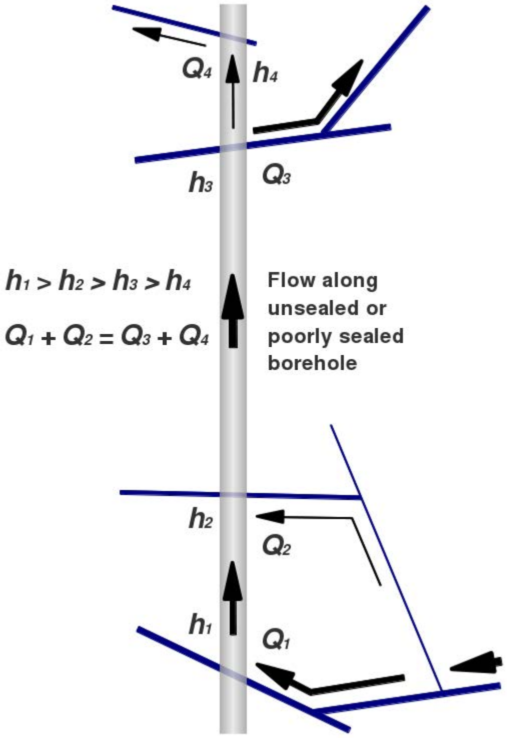

Figure 6. Schematic illustration of possible interactions of an unsealed or imperfectly sealed borehole with a discrete-fracture network in the bedrock, for a case where the hydraulic head gradient is upward along the borehole. For an unsealed borehole where the flow resistance along the borehole is negligible compared to the flow resistance in the fractures, the inequality $h_1 > h_2 > h_3 > h_4$ may effectively approach the case of equilibrated heads, $h_1 \approx h_2 \approx h_3 \approx h_4$.

levels, gradual changes in land elevation relative to sea level, and overland flow from inland areas.

Over longer time periods of concern for repository safety assessments, up to and including continental glaciation cycles, additional processes can be important. These processes include shoreline retreat and evolution of bays, lakes and wetlands, permafrost formation and related processes, advance of continental glaciers, long-term changes in sea level and salinity, and formation of glaciofluvial systems with consequent sediment deposition and/or erosion.

Hydrogeological models necessarily use simplified mathematical constraints (boundary conditions) to represent the consequences of these surface processes, but over time the level of realism has increased.

2.4.1 Elementary boundary conditions

Hydraulic boundary conditions at the surface are often prescribed using some combination of the following:

- specified-head (or pressure) boundary
- specified-flux boundary
- infiltration boundary

For repository study sites in crystalline bedrock sites in Nordic climates and similar situations, a specified-head condition with head equal to the topographic elevation z:

$$h \;=\; z \tag{32}$$

is often used for terrestrial areas, justified by the observation that groundwater levels are close to the ground surface for most of the year (*e.g.* Tóth, J. and Sheng, G., 1996; Voss and Provost, 2001, Follin and Svensson, 2003). A "damped" version of topographic heads:

$$h \;=\; az, \quad 0 < a \le 1 \tag{33}$$

is also sometimes used (usually with the constant a in the range 0.5 to 0.9), reflecting the observation that heads in upland areas tend to be somewhat depressed relative to topography. The portion of the upper surface corresponding to the seabed is either assigned a fixed head $h = 0$, representing constant sea level, or – in variable-density models – a pressure value representing the weight of the seawater column per unit area of seabed:

$$p \;=\; -\rho_w g z \tag{34}$$

Specified-flux boundary conditions are sometimes used in models for which the water table is expected to deviate from topography (for example, drawdown due to a repository in the operating phase). In such cases the specified flux is usually related to precipitation minus evapotranspiration.

A generally recognized problem with specified-flux boundary conditions is that these can lead to excessive heads at the surface of the model (exceeding elevation) in areas with relatively impermeable bedrock. Hence more sophisticated "infiltration" boundary conditions have been implemented in some models, where excess heads at the surface result in re-routing of flux to lower-topography areas or outflowing streams. In the most sophisticated versions, such as the MIKE SHE model (as applied by Bosson et al., 2008; 2010), the re-routing of excess flux is modeled by explicit modelling of surface hydrologic processes, but in models that are more focused on the details of deep groundwater flow, simpler and less physically realistic assumptions may be used.

The CONNECTFLOW model (Follin et al., 2007) implements an infiltration condition in terms of an iteratively calculated flux R that is either in or out of the ground, depending on whether the calculated head h at a point is above or below the time-dependent elevation $z(t)$ of the point:

$$R \;=\; \left\{ \begin{matrix} R_p \quad , & h \le z - \varepsilon \\ -R_p\left(h - z\right)/\,\varepsilon, & h > z - \varepsilon \end{matrix} \right\} \tag{35}$$

where e is a small distance (2 cm in simulations for Forsmark). The second expression ensures that discharge flux will be just enough to lower heads to the surface elevation, in discharge areas. For improved convergence in Newton-Raphson iterations, the continuously differentiable function:

$$R \;=\; R_p\left[\exp\left(\frac{h - z}{0.5}\right) - 1\right] \tag{36}$$

was used in place of the preceding expressions (Follin *et al.*, 2007, p. 95).

2.4.2 Seasonal and diurnal variations

Surface hydrologic conditions at coastal sites around the Baltic Sea go through seasonal as well as daily cycles (Figure 7). While tidal effects on the Baltic are negligible, storm surges driven by wind and/or atmospheric low-pressure systems can produce local sea-level changes which, for example at Forsmark, are significant enough to produce brackish-water input to lakes that are normally 1 m to 2 m above sea level.

Precipitation varies strongly on a daily and even hourly basis during storm events. The main hydrogeological influence of precipitation that falls as snow during the winter may be delayed for weeks or months until the snow melts during warmer weather, with peak melting in early spring. Thus the periodicity of meteoric water flux into the groundwater system has different characteristics in the winter vs. other parts of the year.

Evapotranspiration (both potential and actual) shows a strong seasonal variation as well as daily fluctuations. At the Forsmark site, potential evapotranspiration can be close to zero for the months of October through January, then increases to peak values in late spring and summer (Bosson et al., 2008, Figure 2-4). During the warm part of the year, potential evapotranspiration can vary by close to an order of magnitude, over the span of a few days, due to changes in weather-related factors (temperature, humidity, and cloud cover). Diurnal fluctuations in evapotranspiration are also seen in the spring and summer months.

The influence of these complex seasonal, day-to-day, and diurnal cycles is evident in water-level monitoring data from shallow boreholes (e.g. as presented by Johansson, 2008), and may propagate as pressure signals to deeper boreholes. The effects on flow at repository depths are likely minimal, due to the low conductivity of the bedrock. However, stronger cyclic movements of water in the shallow subsurface could affect advection and dispersion of radionuclides at the geosphere-biosphere interface.

Records of precipitation and potential evapotranspiration for a three-year period have been applied as part of the upper boundary condition for a MIKE SHE model of surface hydrology and shallow hydrogeology, which includes a simplified, continuum representation of the bedrock to repository depths (Bosson et al., 2008; 2010). A similar model, ECOFLOW, has been used for comparative simulations of surficial and shallow hydrologic processes, notably including the effects of freeze-thaw cycles during cold portions of the year (Sokrut et al., 2007). These effects have thus far not been represented in more detailed hydrogeologic models of the deep bedrock.

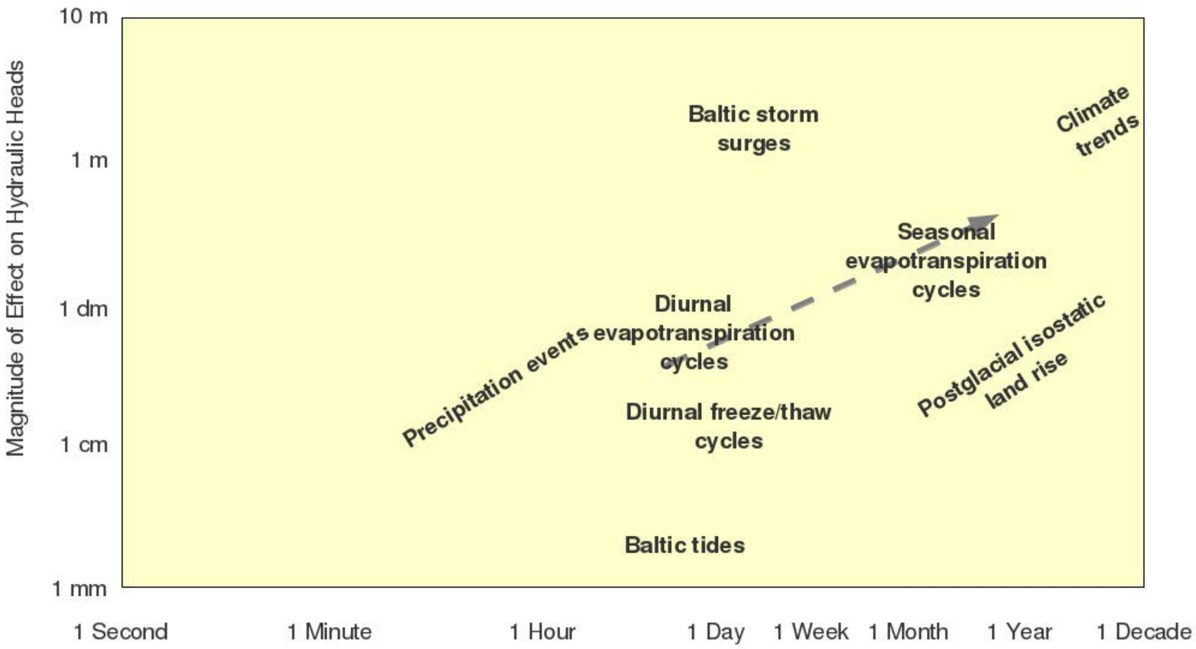

Figure 7. Approximate time scales for conditions affecting the upper boundary of hydrogeological models in the Baltic region.

2.4.3 Surface waters and evolution

Surface waters include the sea (brackish in the case of the Baltic), flowing freshwater channels (rivers, streams, *etc.*) which may be seasonal or ephemeral, particularly in the case of streams draining small catchments, and non-flowing freshwater bodies (lakes, ponds, marshes, bogs, *etc.*). All of these are expected to evolve over the time scales of thousands of years such as are considered in safety assessments.

The surface hydrologic and shallow hydrogeologic model for Forsmark (Bosson et al., 2008) using the MIKE SHE code includes an explicit model for overland flow (based on a 2-D finite difference diffusive wave approximation), which is coupled to the shallow groundwater model (unsaturated and saturated zones), as well as to a module that simulates river hydraulics for in-channel flows. Water levels in ponds and lakes are allowed to respond as ponding results from temporal variation of precipitation and evapotranspiration in combination of the other hydraulic processes (groundwater infiltration, overland flow to channels, and channel hydraulics). The ability to reproduce observed lake levels for the current temperate climate is used as a criterion for model calibration.

The sea is also treated as a dynamic body of surface water in the MIKE SHE model. However, as described by Bosson et al. (2008), it is represented as a "gravel" layer of very high hydraulic conductivity, in order to avoid numerical instability that can result when very large bodies of overland flow are included in the model. This "sea-gravel" layer is assigned a flat topography corresponding to the minimum sea level (for the simulation period). Higher water in the littoral zone during high-sea level events is modeled as overland flow, above this "sea-gravel" layer.

Simpler representations of surface waters are normally used in hydrogeologic models that are focused on flow in the deep bedrock (e.g. Follin et al., 2005, Hartley et al., 2006b,c). The sea is usually implemented as a specified-head or specified-pressure boundary condition, with methods as discussed in Section 2.4.1. Coastal recession is simulated by shifting the area over which these boundary conditions are imposed, in successive time steps.

Lakes are most often simulated as areas with specified heads equal to the lake surface elevations, although in a few cases, surface-water routing schemes have been used to allow lakes to respond dynamically to the local water balance (e.g. Holmén and Stigsson, 2001). As discussed in Section 2.3.1, in a large-scale modelling study of the NE Uppland region that includes Forsmark, Holmén et al. (2003) applied a no-flow boundary condition to the base of lakes to test the effect of an impermeable layer of clay/gyttja (but with specified heads equal to lakeshore elevation at the lake perimeters), but found that this had only a minor effect on regional recharge/discharge patterns.

Over time, lakes around the Baltic coast are expected to be affected by continuing land rise (affecting hydrologic base levels), sedimentation, and accumulation of plant materials, resulting in a transition to marshes, then wetlands, and eventually ordinary terrestrial soils. These processes and related aspects of landscape evolution have been modeled in special-purpose models by Brydsten (2006) and by Brydsten and Strömgren (2010). However, these models have not been integrated into bedrock hydrogeology models.

2.4.4 Periglacial conditions

The term, "periglacial," is broadly defined to mean "an environment of frequent freeze-thaw cycles and deep seasonal freezing," or more narrowly as, "a permafrost environment" (Slaymaker, 2009, following French, 2007). Hydrogeologically important aspects of periglacial environments include (McEwen and de Marsily, 1991; Vidstrand, 2003):

- development of permafrost which acts as a barrier to fluid flow in the shallow subsurface;
- development of taliks which can connect unfrozen ground at depth to the surface;
- formation of saline pockets of groundwater by salt exclusion during freezing.

Modelling of periglacial conditions at Forsmark using the surficial hydrologic model (Bosson *et al.*, 2008) has included cases with permafrost extending from the ground surface to two different depths (100 m and 240 m). To mimic the effect of frozen ground, hydraulic conductivity was reduced. "Through" taliks (taliks that penetrate the full thickness of the permafrost) are modeled (Bosson *et al.*, 2008, p. 46) as forming either below shallow lakes (average depth 0.5 m) for which the lake radius exceeds the permafrost thickness, or below deeper lakes (average depth 4 m) for which the lake radius is at least

1.6 times the depth of the permafrost. Lakes are identified based on water depths computed with the overland flow module. To maintain consistency with the fact that precipitation falling as snow does not contribute to overland flow until temperatures rise above freezing, the delayed release of water from melting snow is simulated by setting a high resistance to overland flow (Bosson *et al.*, 2008, p. 64); similar artificial parameter adjustments are used to mimic unsaturated-zone behavior during freeze-thaw periods.

2.4.5 Glacial conditions

Hydrogeologic effects of glaciation depend on basal conditions of the glacier, as described by Provost *et al.*, (1998).

For "cold-based" glaciers advancing over permafrost, there is little possibility for glacial meltwater to infiltrate. The weight of the glacier (up to 2 km thick) further compresses the bedrock and is expected to result in closure of many fractures, particularly subhorizontal fractures in the shallow bedrock. Due to the fracture hydromechanical properties discussed in Section 2.1.4, the hyperbolic relationship between stress and fracture stiffness implies that the sensitivity of fracture transmissivity to changes in stress during glacial loading will be highest in the shallow bedrock.

The insulating effect of thick ice cover, combined with the earth's natural geothermal flux, eventually leads to thawing of permafrost below a glacier, so that a "warm-based" condition is achieved. Liquid water may also form at the base of glaciers due to pressure/solid-liquid phase change relationships. This water is under high pressure (possibly as great as the weight of the ice column), forming recharge areas from which groundwater flows toward areas with lesser ice overburden.

The most extreme hydraulic situations potentially occur during glacial retreat when a high hydraulic gradient exists across the retreating face of the glacier. To some extent, basal pressures may be relieved by subglacial fluvial systems. However, modern and Pleistocene examples of jökulhlaups demonstrate that basal meltwater pressures do sometimes reach levels that are sufficient to lift and break up ice dams on glacial meltwater lakes.

Provost et al. (1998) represented these circumstances in terms of a no-flow condition at the base of cold-based glaciers, and a specified pressure head equal to the ice thickness, for warm-based and glacial retreat situations. More recent models have used similar assumptions for boundary conditions.

Holmlund (2008) has discussed factors that might influence hydraulic head gradients near the edge of a glacier. For a cold-based, advancing continental glacier, physical modelling indicates a cold frontal zone with a gradually warmer base as the ice thickens away from the front. Evidence from Greenland (Zwally et al., 2002) indicates that ice velocities respond to surface melt, at the glacial front and inland to where the ice is 1000 to 1500 m deep. This suggests that surface meltwaters collecting in supraglacial lakes (moulins) or in crevasses can influence water pressures at the base of glaciers, despite that in the interior of such glaciers, the ice is below freezing. Thermomechanical modelling of meltwater-driven crevasse propagation by Alley et al. (2005) indicates that this is physically plausible mechanism to produce this effect. In such a system, it should be expected that the hydraulic head for meltwater infiltrating at the base of glaciers will be regulated by the elevation of meltwater ponding in moulins and crevasses, resulting in hydraulic heads that are well below the mean surface elevation of the glacier.

2.5 Lateral and basal boundary conditions

Lateral and basal boundaries of site-scale models require assumptions regarding the effective conditions at depth, since in general it is not possible to characterize them directly. Hence relatively simple boundary conditions are usually assigned to these boundaries, justified by arguments that these boundaries are placed far enough from the domain for which results of importance are sought, that the results are controlled by the more well-understood surface boundary conditions. This argument is sometimes strengthened by the use of nested models, which by using a coarser resolution for the outer domain(s), allow lateral and basal boundary conditions to be imposed even farther from the domain of concern.

2.5.1 Elementary boundary conditions

The two types of boundary conditions that are usually used for lateral/basal boundaries are:

- specified head, and
- specified flux.

When specified-head conditions are used, these are normally based on regional topographic gradients. Using this type of boundary condition allows for the possibility that regional-scale flows, driven by regional topography, can contribute significantly to site-scale flow. As shown by Voss and Andersson (1991), regional flows can be significant, at least in homogeneous bedrock. Large-scale flow modelling with more heterogeneous models of the bedrock, and/or fine-scale topography, leads to doubts about the generality of this conclusion (Ericsson et al., 2006). However, for safety assessment it is often conservative to assume that regional gradients can contribute to flow through a repository.

Specified-flux boundaries on the lateral/basal sides of groundwater flow models are most commonly implemented as no-flow conditions. A no-flow condition may be defensible for the seaward boundary in models that extend for some distance over the sea floor, as head gradients to drive flux should tend to zero offshore. A no-flow condition may also be justified as the basal condition, due to both a tendency for hydraulic conductivity to decrease with depth, and the presence of deep saline brines which impede penetration of fresh waters.

Along other sides of a model, no-flow conditions are sometimes justified by arguments that the edge of the model is parallel to the regional hydraulic gradient, or that it is aligned with a surface-water drainage divide. These two conditions may not necessarily be adequate to ensure a no-flow boundary at depth, and preferably should be defended by sensitivity studies.

2.5.2 Nested regional/local models

Nested regional and local models provide a means for shifting assumptions about lateral/basal boundary conditions farther from the domain for which flow predictions are needed, by interposing a coarser-resolution (and hence less computationally expensive) regional submodel between the local/site-scale model and the edges where boundary conditions are applied. Such models may be directly coupled to ensure continuity of head and flux at the interface between modelling scales, or indirectly coupled by applying data from regional-scale calculations to the boundary of the local model. If indirect coupling is used, additional checks of consistency between the regional and local domains are usually needed to ensure confidence in the results.

Current trends favor the direct-coupling approach, for situations where a single software application can represent all relevant processes. Examples include the CONNECTFLOW application for repository-scale simulations of a repository layout for Laxemar (Hartley et al., 2006b, p. 112), where a detailed DFN model of the repository volume was directly coupled to a regional-scale ECPM model. CONNECTFLOW also permits embedding continuum porous-medium (CPM) representations (e.g. of backfilled repository tunnels) in a DFN model, which could in turn be coupled to larger-scale, nested CPM models.

2.6 Initial conditions

Initial conditions need to be prescribed for models of transient flow situations, such as:

- Drawdown of groundwater during repository construction,
- Resaturation of a repository following closure,
- Simulation of the long-term evolution of density-dependent flow which is affected by palaeohydrological changes in groundwater salinity.

The first case is an example of a transient flow situation that begins from approximately steady-state conditions. The initial condition is ordinarily obtained from a steady-state flow simulation to approximate equilibrium conditions, at least in the case of sites that are not affected by long-term density-dependent transients.

The second case is an example of a transient flow situation that follows another transient situation. A multi-step simulation would normally be used, starting with a steady-state calculation of equilibrium conditions. Hence, for this and the first case, physically plausible initial conditions can be calculated rather than simply assumed.

When long-term transients in fluid density are significant due to palaeohydrological effects, then establishment of appropriate initial conditions is difficult. For simulations of the long-term evolution of groundwater at Forsmark, Follin et al. (2007) assumed an initial condition at 10,000 year BP, in which water in the rock matrix was a mix of two reference waters (either Holocene or old-meteoric/glacial water and deep saline water), while water in the fractures was a mix of three reference waters (Holocene glacial melt water, old meteoric/glacial water and deep saline water), with linear gradients in the fractional composition of both fracture and matrix water (Figure 3-67, Follin et al., 2007, p. 99).

Self-consistent initial conditions for such situations could possibly be obtained by running the models through a reference glacial cycle, and then using the resulting distribution of groundwater types as the initial condition for simulations of the subsequent glacial cycle. This has been suggested (Chapman et al., 2010) but has not been done in practice.

3 Examples from site-specific applications

Research on methods for hydrogeologic modelling of crystalline hard rock was spurred in the 1970s by interest in geothermal energy as well as exploitation of sparsely fractured crystalline rock for radioactive waste disposal (Witherspoon, 2000). The resulting course of development of field-scale modelling methods, through the early 1990s, is summarized by National Research Council (1996, p. 307-404). Important research sites included the Fanay-Augere mine in France, the Chalk River Site in Ontario, Canada, the Stripa mine in Sweden, the Canadian Underground Research Laboratory (URL) in Manitoba, Canada, and the Grimsel site in Switzerland. Model developments for the last three of these sites, along with more recent developments at other sites, are summarized in the following sections.

3.1 Stripa, Sweden

The Stripa research site in Sweden (Fairhurst *et al.*, 1993) was situated in granite adjacent to a former iron ore mine. During the period of operations 1976-1992, research drifts were developed over a distance of a few hundred meters into the granite, at depths ranging from 330 m to 360 m, with complementary geological investigations mainly at depths of 310 m to 410 m depth. Hydrologic conditions at the site were highly disturbed due to proximity to the iron mine, which had been in operation for several hundred years. Efforts to relate models to surface hydrologic conditions were minimal.

One important model application at Stripa was a 3-D conditional DFN model for flow and transport (Dverstorp and Andersson, 1989). This model was applied on a tunnel scale of approximately 75 m. Fractures were simulated conditionally to reproduced mapped traces on the tunnel, while honoring fracture statistics. The model considered saturated flow in discrete fractures, and used idealized boundary conditions (specified heads) on the exterior of the model volume, with approximately radial flow to the tunnels at atmospheric pressure. Further development of this numerical model (but in smaller, block-scale simulations) by Nordqvist *et al.* (1992) incorporated the concept of aperture variation within fractures, which gives rise to dynamic flow channeling within fractures; this model was motivated by anomalous results of tracer migration experiments in the Stripa 3-D migration experiment, as described by Witherspoon (2002).

Slightly larger-scale DFN models were applied in the Site Characterization and Validation (SCV) experiment (Olsson, 1992). These included comparisons of models developed by four different modelling teams, using different conceptual and numerical models of fracture networks. The models were developed based on fracture data from tunnels and calibrated based on hydraulic tests in boreholes. In an initial exercise, the models were used to predict inflows to a “simulated drift,” consisting of parallel boreholes drilled along the perimeter of a tunnel which was then excavated so that flows to the open drift could also be measured and compared with models. Saturated conditions were assumed, and simple boundary conditions (hydrostatic heads) were applied to the outer boundaries of the models.

As discussed by NRC (1996), the results showed that predictions broadly similar to eventual results could be obtained by a variety of discrete and continuum implementations, provided that major fracture zones were included deterministically in the models, and calibration to available hydrologic data was performed. Important practical developments from the project included methods for representing fracture zones deterministically, and for calibrating with respect to wellbore testing methods (Dershowitz *et al.*, 1991; Herbert and Lanyon, 1992). A unique “simulated annealing” approach for stochastic inversion of hydrologic data, based on 2-D lattices embedded in planes that represented the

3-D connections among major fracture zones (Long *et al.*, 1992; Mauldon *et al.*, 1993), was applied to the SCV experiment but has not seen subsequent practical application.

3.2 Grimsel Test Site, Switzerland

The Grimsel Test Site came into operation in 1983. This underground research laboratory was located in granite of the Central Aar Massif, at a depth of 450 m below the slope of the Juchlistock, at Grimsel Pass in the Central Alps of Switzerland.

Much of the modelling effort at Grimsel has focused on detailed-scale models (less than 1 m to a few tens of meters) in order to investigate of fundamental processes such as gas migration, radionuclide retention, and colloid transport (*e.g.* Kosakokowski and Smith, 2004).

Hydrogeological models that have been developed in support of this work have focused on a few transmissive structures, on a detailed scale. One shear zone was investigated with 8 boreholes that were drilled to intersect the shear zone at distances of 3 to 16 m from the tunnel wall. Hydraulic models of this zone included a 2-D heterogeneous continuum model (Herzog, 1989) and a geostatistical 2D inverse model (Meier *et al.*, 2001) which was used to elucidate the distribution of transmissivity within the part of the structure that was characterized by borehole testing.

A notable outcome of work at Grimsel was a focus on detailed, geologically based descriptions of the hydrogeological properties of fractures and shear zones (Martel and Peterson, 1991; Bossart *et al.*, 1991; Mazurek *et al.*, 2001). This brought out the potential importance of shear zone internal structure including breccias and fault gouge. This work forms the basis for complex fracture models (Doughty and Tsang, 2003).

3.3 Whiteshell Underground Research Laboratory, Manitoba, Canada

The Whiteshell Underground Research Laboratory (URL) was located in Archean granite of the Lac du Bonnet Batholith in southeastern Manitoba, at the western edge of the Canadian Shield. The URL was in operation from 1984 until the early 2000s, when it was decommissioned. The main working levels of the facility were at depths of 240 m and 420 m.

The site turned out to have very few hydraulically conductive fractures at the deeper levels. A series of gently-dipping fracture zones which have been interpreted as thrust faults are the most significant features identified for hydraulic modelling (Davison *et al.*, 1996). Sub-vertical fractures were found to be ubiquitous in the shallow bedrock, but rare or absent below the primary gently dipping fracture zone, which was named FZ2. Below FZ2, hydraulically connected fractures were extremely scarce, except for as fractures which were interpreted as being related to downward splays of FZ2. Anomalously high horizontal stresses were encountered in the rock below FZ2, which is consistent with the idea of high-strength, relatively unfractured rock acting as a rigid body below more pervasively fractured rock.

Due to the sparsity of conductive fractures at depth, hydrogeological characterization and modelling focused on a deterministic description of the main fracture zones, including investigations of heterogeneity within FZ2. Hydrogeological testing revealed permeabilities ranging over six orders of magnitude within FZ2, with indications of channeling at the site scale. One of these site-scale channels followed the intersection of FZ2 with one of its major splays, while others were interpreted as being a result of structural controls (related to undulations in the fault surface) or hydrogeochemical phenomena (*e.g.* precipitation of minerals due to mixing of groundwaters with dissimilar chemistry).

Srivistava (2002) developed a regional-scale discrete model of faults based on geostatistical, probabilistic simulation of propagation of surface lineaments to depth. This model utilized surface expression of fractures, statistics on fracture density and length distributions, structural geological principles for down-dip behavior of fractures, and truncation rules due to regional tectonic and geologic considerations. The approach compensated statistically for areas with overburden cover or weak contrast in aerial photography.

The concepts developed in this model might be applicable to site-scale, conditional simulation of sub-kilometer-scale, minor deformation zones, *e.g.* based on detailed magnetic and/or LIDAR (airborne laser-ranging) surveys.

Sykes *et al.* (2003) analyzed the regional-scale flow system in a hypothetical plutonic setting, 6000 km2, 1.5 km deep, based on data from Whiteshell Research Area and the URL in Manitoba. This model represented topography, hydraulic properties distribution *e.g.* permeable fracture zones (based on the model of Srivistava, 2002), relationships between fracture zone permeability and depth, long-term influence of shield brines, and assessment of glacial impact based on a glaciation model (Peltier *et al.*, 2000). For temperate conditions, Sykes *et al.* (2003) treated the water table as a subdued replica of the topographic surface, with water table divides roughly corresponding to surface water catchment boundaries. The approach was applied to an approximately 130 km^2 subregional domain with low topographic relief (elevation range of 350 m to 410 m), with wetlands and lakes along with creeks, streams and rivers. Many streams/rivers in the area were linear and suggestive of underlying fracture zones (Srivistava, 2002).

Park *et al.*, (2008) performed further hydrogeologic modelling, applying the "lifetime expectancy" concept of Cornaton *et al.* (2008) as a performance measure for a hypothetical repository in this Canadian Shield environment. They considered effects of geometric and hydraulic characteristics of the fracture zones in a subcatchment of the regional domain modeled by Sykes *et al.* (2004), with up to 1000 major and intermediate fracture zones, based on surface lineament analyses and subsurface studies (Srivistava, 2002). Groundwater salinity was noted to increase with depth in the deep shield (up to 1.3 kg/L), and was attributed to either marine intrusion or rock-water interaction.

The numerical model used by Park *et al.* (2008) was FRAC3DVS (Therrien and Sudicky, 1996; Therrien *et al.*, 2003). This simulates variably saturated groundwater flow and reactive transport, and is able to simulate flow and transport in zoned-type porous or dual porosity/dual permeability media. For simulations on the subregional scale, the "fractures" (representing fault zones or fracture zones) are represented as 2-D planar features, while the "matrix" (representing less permeable fractured rock) is modeled in 3-D.

Values of porosity and permeability for the rock matrix in this model were assumed to be anisotropic, with depth-dependent magnitude and anisotropy. A statistical model for depth-dependent permeability in fracture zones was based on data from the Whiteshell Research Area. A lognormal distribution was used for fracture zone width (thickness), with generic rules for porosity as a function of permeability in the zones.

Only saturated groundwater flow was considered, based on generally shallow depths of water table in the area in the Canadian Shield setting. A specified-head boundary condition was used for lakes, wetlands, and rivers. A recharge rate of 1.0 mm/yr applied to remaining top surface of the model (estimated by applying a specified-head boundary condition equivalent to surface elevation to the entire upper surface, and averaging total recharge into the domain over the top surface of the model). Bottom and side boundaries along surface water catchment boundaries were modeled as impermeable (no flow). The solution obtained was for steady-state flow. Results were presented in terms of head and Darcy flux distributions, plus mean lifetime expectancies for water molecules released from a given point which were computed by steady-state backward-in-time transport equation (Cornaton *et al.*, 2008).

A recent modelling effort (Lemieux and Sudicky, 2010), covering the same area, has been used to study the impact of the Wisconsinian glaciation on the Canadian continental groundwater flow system in terms of groundwater age (residence time). The model represents key processes affecting coupled groundwater flow and glaciation: density-dependent flow, hydromechanical loading, subglacial infiltration, glacial isostasy, and permafrost development. Notably, this model yields a finding that subglacial meltwater mixing with older groundwaters below the ice can infiltrate to depths of up to 3 km, depending on the permeability of the subsurface rocks, the presence of dense brines, and the presence or absence on deep fractures or conductive faults.

3.4 WIPP site, New Mexico, USA

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, USA, since 1999 has been an operating repository for transuranic wastes produced by nuclear weapons research and production. As described by Meigs and Beauheim (1997), the facility is constructed in bedded, Permian-age halites which are overlain by an approximately 7 m thick layer of fractured dolomites, which in turn are overlain by clastic-dominated, continental deposits. Thus the site is in evaporite and clastic deposits, rather than crystalline hard rock. However, a few aspects are relevant for describing the state-of-the-art for site-scale hydrogeologic modelling in fractured rock.

A major innovation from this site has been the development and use of a “pilot-point” methodology (RamaRao *et al.*, 1995; LaVenue *et al.*, 1995) to model spatial variability of the Culebra dolomites. This is a method for conditional simulation of transmissivity that preserves geostatistical measures of the spatial correlation structure, but also honors the measured transmissivity values at each of the numerous wells where measurements are available for this site. Multiple simulations (up to 100) of the Culebra dolomite transmissivity variation are used to evaluate the consequences of residual uncertainty associated with heterogeneity of this formation. The method is implemented in the GRASP-INV code which has been used to meet WIPP’s requirements for ongoing regulatory compliance certification, incorporating new information as it becomes available (Meigs and Beauheim, 1997).

Investigations of multi-scale transport properties of the Culebra dolomites also led to development of single-well injection-withdrawal (SWIW) testing, and evaluation of these using multi-rate models for mass transfer (Haggerty and Gorelick, 1995; Meigs and Beauheim, 1997). These methods have since been applied for characterization of bedrock transport properties at repository sites in Sweden.

3.5 Äspö Hard Rock Laboratory and Simpevarp-Laxemar site, Sweden

The Äspö Hard Rock Laboratory (HRL) is located below the island of Äspö in Sweden’s Baltic coastal archipelago near Oskarshamn. The laboratory’s working levels range from about 320 m to 420 m depth. The host rock is primarily granite or granodiorite of variable composition. The laboratory has been used for a variety of experiments to test and demonstrate components of the KBS-3 disposal concept, including buffer and backfill experiments, investigation of the EDZ formed by controlled drill-and-blast tunnel excavation methods, a comparison with an alternative method of excavation using a full-face tunnel boring machine (TBM), and a series of tracer experiments (the Tracer Retention Understanding Experiments, or TRUE) to demonstrate and understand the capacity of the bedrock to retain radionuclides. Overviews of the investigations are given by SKB (1996) and Olsson (1998).

The island of Äspö is separated by narrow, sheltered straits from the Simpevarp peninsula and island of Ävrö to the south and east, which together constitute the Simpevarp subarea, and the Laxemar subarea; both Simpevarp and Laxemar were investigated as a repository candidate sites, with Laxemar becoming the focus of more detailed investigation after Simpevarp was discarded early in the process. An overview site investigations and their outcomes in terms of site descriptive models are summarized by (SKB, 2008a; SKB, 2005A; SKB, 2009).

Considering the proximity of the Simpevarp and Laxemar sites to the Äspö HRL, their similar geology and closely related hydrogeological settings, their significance for the state-of-the-art in hydrogeological modelling of crystalline hard rock can be discussed as a single locale for which investigations and model development were fairly continuous from the late 1986 through 2011.

Significant developments of hydrogeological modelling methods from the Äspö HRL, Laxemar, and Simpevarp have been mentioned as examples throughout Chapter 2 of this report. Here a few of the main developments are briefly summarized.

An international modelling task force performed a series of model predictions and evaluations, prior to and during the construction of the HRL. The Äspö Task Force (Dershowitz *et al.*, 2003; Rhén and Smellie, 2003) yielded practical experience in application of surface boundary conditions to site-scale hydrogeological models of sparsely fractured, crystalline hard rock, and integration of hydrogeochemical information with groundwater models. Development and application of models for density-dependent flow led directly to the DarcyTools model (Svensson *et al.*, 2004) which has seen subsequent application in the site investigations and predictive modelling for the Laxemar and Forsmark candidate repository sites. Modelling of the TRUE experiments (Poteri *et al.*, 2002) in the HRL spurred development of smaller-scale flow and transport models for crystalline hard rock, including models of complex fracture effects.

Initial DFN models of the bedrock at Äspö based on scanline mapping along narrow exposures (2 m wide cleaned “trenches”) were found to give a poor representation of bedrock hydraulic conductivity, which resulted from a population of extensive discrete fractures that were poorly represented by lognormal fracture size distributions. Recognition of the importance of these sparse but extensive fractures led to suggestion of power-law distributions for fracture size which were initially applied in DFN models for another Swedish study site (Geier *et al.*, 1992), but have since been adopted for the Laxemar-Simpevarp area as well as numerous other sites in crystalline hard rock. Some of the extensive fractures at Äspö could be traced either as single fractures or échelon fractures for 25 m or more (Geier, 2005). Similar echelon features were also found using LIDAR (airborne laser-ranging) surveys as part of the Minor Deformation Zone project within the Laxemar site investigations (Olsson *et al.*, 2007). Anisotropic flow properties of diabase dikes (acting as low-permeability barriers in the transverse direction, but high-permeability flow zones in the parallel direction due to fracturing in the contact zone) has also been suggested by field investigations at Laxemar.

The dataset from the preliminary, surfaced-based investigations for the Äspö HRL was also used by the Swedish regulatory authorities for the SITE-94 safety assessment study (SKI, 1996), which was an exercise in evaluating the safety of a hypothetical repository, based exclusively on surface-based data such as would be available for the first stage of licensing (construction license application) for a spent-fuel repository in the Swedish regulatory framework. Site-scale models based on a stochastic continuum approach (Tsang *et al.*, 1996) and a discrete-feature modelling approach (Geier, 1996) were used to investigate the effects of heterogeneity on multiple scales, as well as conceptual and interpretation uncertainties that result from approaches taken by different modelling groups for the same data. The discrete model led to predictions of groundwater travel times on the order of 10 to 50 years for some waste package positions, faster than had been typically predicted by equivalent continuum models at that time.

Regional-scale simulations of a glacial scenario using a coupled density-dependent flow and transport model (Provost *et al.*, 1996) highlighted the possibility of very high head gradients that could drive infiltration of oxygenated or dilute glacial meltwaters during glacial retreat. When equivalent heads calculated from this regional model were applied as boundary conditions to the site-scale discrete-feature model of Geier (1996), this led to an indication that these glacial meltwaters could reach repository depths on time scales of a few years.

1-D reactive transport modelling by Glynn *et al.* (1999) suggested that such rapid penetration times could lead to oxygenated water reaching repository depths. This suggestion has been discounted based on calculations which indicate that oxygen would ordinarily be consumed by, *e.g.*, decaying organic matter in the shallow subsurface, or by reactions with biotite, sulfides, or other minerals in the bedrock. However, recent reactive transport modelling for a Canadian Shield setting (Spiessl *et al.*, 2008) suggests that the question is not fully resolved. The risk of dilute glacial meltwaters at repository depths leading to bentonite buffer erosion is more broadly accepted (*e.g.* SKB, 2006) and has motivated further investigations of the possible extent and impacts on a KBS-3 system (SKB, 2011).

On a larger scale, the Oskarshamn area that includes Laxemar, Simpevarp, and Äspö has been the focus of regional- and superregional-scale hydrogeological modelling to investigate the role of topography, computational mesh resolution, and other factors on the persistence of regional flow systems in a Fennoscandian Shield setting (Voss and Provost, 2001; Ericsson *et al.*, 2006; Ericsson *et al.*, 2010). Results point toward a strong influence of local topography and subvertical deformation zones on flow circulation at depth.

3.6 Forsmark candidate site, Sweden

The Forsmark candidate site is located along the Baltic coast in northern Uppland, Sweden. The investigations (as summarized by SKB, 2008b) have focused mainly on the bedrock within a “tectonic lens” formed by subparallel, regional ductile-brittle fault zones and subordinate structures. Within this lens, the bedrock is dominantly a medium-grained metagranite which has been affected by penetrative ductile foliation at mid-crustal depths and under high-temperature metamorphic conditions.

A few smaller, subvertical deformation zones cross the lens, but according to the site descriptive model (SKB, 2008c) are considered to be of minor importance relative to a stack of gently SE-dipping deformation zones. The target volume for the candidate repository is in the footwall of the lowest zone in this stack of deformation zones, and is very sparsely fractured. In this sense, the site is similar to the Canadian Whiteshell URL site (Section 3.3). Like that site, there have been indications of anomalously high stresses in the footwall rock, although the evidence has been less conclusive.

Investigations and hydrogeological modelling of the Forsmark site have used largely the same methods as for the Simpevarp and Laxemar sites. Major differences include (1) the very sparse fracturing at repository depths at Forsmark, (2) early recognition of strong structural control on fracture domains, and (3) an extremely high-transmissivity, “shallow bedrock aquifer” consisting of subhorizontal sheet joints in the uppermost 100 m to 150 m of the bedrock. Relatively rapid post-glacial isostatic rebound, together with gentle topography, also implies hydrologic boundary conditions which change more rapidly with time, due to retreat of the Baltic as the present coastline rises (Follin, 2008).

In part due to the long-term transient groundwater conditions created by relatively rapid coastal recession, one of the major developments in hydrogeological modelling methodology for the Forsmark site (also carried over to the Laxemar site) has been the use of hydrogeochemical interpretations in combination with simulations of “reference waters” in coupled density-dependent flow and transport models, as a means of model calibration and validation (Follin *et al.*, 2008). While this has been a significant development in terms of modelling technology and methodologies, the application to Forsmark has been limited by practical difficulties in obtaining reliable geochemical samples from the tight rock at depth, particularly “first strike” samples in the early stages of site characterization. The resulting sparsity of the data set leaves some questions as to the significance of discrepancies between models and observations, particularly in terms of the depths at which steep transitions are observed between groundwaters of different chemical and isotopic compositions.

The apparent sparsity of the deep fracture system at Forsmark also leaves open questions as to why there are still a few water-conducting pathways through the rock, outside of the identified deformation zones. In such a fracture system, non-Poisson (*i.e.* uniformly random) spatial organization of the fractures may be important. Exploratory modelling by Geier (2011), using alternative DFN conceptual models that are equally well supported by site data, suggests that this conceptual uncertainty may be significant in terms of the distribution of flows to canister positions, and might not be resolvable until a large fraction of a repository has been constructed.

3.7 Olkiluoto site, Finland

The Olkiluoto site, located on an island along the southwestern Baltic coast of Finland north of Rauma, is situated in Paleoproterozoic high-grade metamorphic rocks of epiclastic and pyroclastic origin, dominantly migmatitic gneisses with lesser occurrences of tonalitic-granodioritic-granitic gneiss and pegmatitic granites. The ductile fabric of the rock is thus more strongly developed than the granitic sites discussed above, with consequences in terms of the distribution of brittle fracture orientations.

Description of the discrete fracture network and hydrogeological modelling of the Olkiluoto site in Finland has been based on similar concepts and even some of the same modelling experts as have been used for the Forsmark and Laxemar sites in Sweden. The geological DFN model (Buoro *et al.*, 2009) is based on a similar set of DFN conceptual models to those for Forsmark and Laxemar. The hydrogeological DFN model has used similar methods for incorporating hydraulic testing data from boreholes, particularly Posiva flow log (PFL) data (Hartley *et al.*, 2009).

FEFTRA software (Löfman *et al.*, 2007) has been used for Hydro-DFN simulations (Hartley *et al.*, 2010) rather than the CONNECTFLOW software that was used by the same group of consultants for the Forsmark and Laxemar sites. The representation of an EDZ along the base of tunnels was similar to the representation used for Forsmark (Hartley *et al.*, 2010, p. 39). One variant to test sensitivity of the Hydro-DFN model to fracture size model was found to be computationally intractable as a pure DFN model, so a nested CPM-DFN model was suggested (Hartley *et al.*, 2010, p. 78).

An update of the site-scale model incorporating discrete deformation zones and a dual-porosity continuum description of the bedrock (Löfman *et al.*, 2009) used dual-porosity/dual permeability representations of both the hydrogeologic (deformation) zones and the intervening, more sparsely fractured bedrock. The hydrogeologic zones were represented in the computational mesh by sets of 2-D triangular elements, which coincided with the faces of 3-D, tetrahedral elements from the discretization of the adjacent sparsely-fractured rock.

The model of bedrock hydrogeological properties is essentially deterministic, although heterogeneity is simulated by kriging interpolation and hydraulic conductivities have been adjusted in some parts of the model to improve the match to hydraulic observations. The outcome is likely a “smoother” hydraulic conductivity field than would be obtained by the ECPM approach that has been used for Forsmark and Laxemar; this could result in more evenly distributed flow lines and less variability in water residence times, than a stochastic modelling approach.

Evolution of the groundwater levels due to drawdown by repository tunnels is simulated using a free-surface approach similar to that used for Laxemar (Svensson, 2006). Salinity/density effects were neglected for these simulations based on an argument that density-dependent flow does not significantly account for drawdown of the water table in the upper part of the bedrock; however it can be noted that this approach does not give insights into the possibility of upconing of deep saline water.

Spatially varying infiltration was accounted for by an *ad hoc* algorithm involving temporarily “switching off” infiltration in successive time steps, whenever the model’s water table elevation rose above observed elevations. Elsewhere a uniform and constant infiltration (influx of meteoric water) is applied. The algorithm was shown to reproduce the measured, undisturbed (*i.e.* pre-excavation) water table to a good approximation provided that sufficiently small time steps were used.

Physical processes that control infiltration and its spatial variation (*e.g.* airborne precipitation, surface runoff, evaporation and transpiration) are not directly accounted for in this bedrock hydrogeological model, but have been modeled separately with a surface hydrologic model (Karvonen 2008; Karvonen 2009). This is similar to the situation for the Forsmark site, although the surface hydrologic model used for Olkiluoto is somewhat less able to represent the influence of shallow bedrock hydrogeological features on near-surface flow, compared with the MIKE SHE-MIKE 11 models of Bosson *et al.* (2008; 2010).

4 Assessment of state-of-the-art

4.1 General trends in model capabilities

Site-scale hydrogeological modelling for repositories in crystalline hard rock requires models that can account for the effects of strong heterogeneity on a wide range of scales, and also account for relevant physical processes that could affect flow and transport.

The conclusions of an international GEOTRAP workshop on representation of heterogeneity in geosphere models (NEA, 2002) included these two comments:

- *Models of groundwater flow are currently available that allow, in principle, a realistic representation of the structural variability of a geologic medium. Availability of data is the most important constraint on the use of these models....*
- *Integrated modelling approaches coupling flow, transport, and chemical reactions appear very promising. The computational tools are still, however, under development and only a few examples of realistic applications are currently available.*

A decade later, at the time of this report, both of these statements are still applicable, but require some qualification.

Capabilities of models to incorporate realistic models of geologic structure have increased significantly over the past decade. However, hydrogeological data are still usually available only from a small fraction of the rock volume that must be considered in site-scale models. Underground access via tunnels (as in ONKALO or in earlier underground laboratories at Grimsel, Äspö, and the Whiteshell URL), gives a high density of data around the tunnels but still leaves large volumes of rock with no direct information. Observations of drawdown due to such facilities show promise as a means of calibrating site-scale models, but examples of calibrations of stochastic representations (rather than deterministic representations) of heterogeneity are still scarce.

Integrated models that couple flow and non-reactive transport are now well established, particularly those based on continuum porous-medium representations. Sites with well-developed examples of practical applications include Laxemar, Forsmark, Olkiluoto, and the Whiteshell URL (on a regional scale). Models that incorporate reactive transport remain mainly in the realm of research tools.

Additional modelling tools that are capable of modelling coupled processes at an equal level of sophistication, but which, to the author's knowledge, have not yet been used for practical applications at repository sites in crystalline hard rock, include:

- FEFLOW (DHI-WASY Gmbh, Berlin, Germany), and
- ROCKFLOW (Leibniz University, Hannover, Germany, www.rockflow.de)

The latter code has additional capabilities for reactive transport and coupled thermal-hydro-mechanical process simulation in fractured rock.

Thus far, no single software application has emerged that allows fully coupled treatment of all relevant processes – thermal, hydraulic, mechanical, and chemical transport processes in the bedrock, together with climate-related physical processes at the ground surface – with explicit treatment of heterogeneity at all relevant scales. Practical applications therefore require combining different models or submodels that incorporate different simplifications. This is exemplified by the CONNECTFLOW software suite which provides multiple ways of interfacing its component DFN and CPM models.

Key areas in which further developments can be expected include:

- Explicit treatment of the unsaturated zone at the upper boundary rather than use of a free-surface;
- More physically based methods for simulating heterogeneous infiltration at the ground surface;
- Improved coupling of bedrock hydrogeological models to surface hydrological models that account for the interactions of overland flow, streams, and lakes with the shallow bedrock;
- Methods for simulating coupled hydromechanical effects, particularly during glaciations, at more realistic levels of detail for the site scale.

According to information given at www.connectflow.com (as of the date of this report) the NAPSAC fracture-flow module of CONNECTFLOW has already been extended to allow more explicit treatment of the unsaturated zone in discrete fracture networks.

4.2 Computational demands of current models

Hydrogeological models of fractured crystalline hard rock, particularly discrete models, are intensive in terms of computational resources, and therefore tend to be limited by computer technology.

For example, the combined CPM-DFN model for the repository block-scale at Laxemar (Hartley *et al.*, 2006b) includes up to 1.47 million fractures in a single realization. Even after simplifications to removing isolated and "dead-end" fractures which do not play a role in steady-state flow, the matrix equations that need to be solved for this model have about 1.95 million degrees of freedom. Even when a supercomputer is employed, such large models can require computation times of many hours to converge to a solution.

In the FEFTRA model of Olkiluoto (Löfman *et al.*, 2009), the mesh for the baseline case consisted of approx. 700,000 nodes and 4 million tetrahedral and triangular elements. Simulations of drawdown due to ONKALO, with additional refinement around the tunnels, led to a mesh with approximately 850,000 nodes and 5.2 million tetrahedral and triangular elements.

For a DFM implementation of SKB's SDM-Site Forsmark site descriptive model and preliminary repository layout (Geier, 2010), coupling a DFN model of the rock around the repository with discrete features to represent the EDZ of deposition tunnels, deposition holes, major deformation zones, and a simplified, effective discontinuum representation of the rock mass on larger scales, the finite element mesh for a typical realization included approximately 2.5 million nodes and 5.8 million triangular elements. This led to a total simulation time of approximately one week for each stochastic realization of the model (including stochastic simulation of the DFN, calculation of fracture-tunnel intersections to simulate adaptation of deposition holes to SKB's deposition criteria, followed by mesh assembly, flow simulations, and particle tracking from each of the deposition holes). These times are using an IBM M55 tower configured with dual Intel Core 2 processors at 2.13 GHz CPU clock speed and 2.9 gigabytes of 667 MHz memory, and Linux operating system.

The dominant part of the process, in terms of computation time, involves set-up and iterative solution of the matrix flow equations. The time needed for this stage scales roughly as N^3, where N is the number of nodes in the finite element mesh.

For models based on stochastic realizations of DFN models, the time required for mesh discretization is also significant, particularly for site-scale ECPM models which require discretization of the DFN realization, followed by many thousands of block-scale flow solutions, to obtain the effective permeability tensors for each block. This has led to practical limitations on the number of stochastic realizations that can be considered within the time span of site-descriptive modelling and safety assessment projects, in some cases as low as just one or two realizations for ECPM models of the Forsmark site (Hartley *et al.*, 2006b), though in more recent applications the number of realizations was increased (Joyce *et al.*, 2010).

In the case of the Hydro-DFN model of Olkiluoto, only a single realization of the Hydro-DFN was simulated for each model variant; this was justified by low variability in a set of 10 realizations for the base case (Hartley et al., 2010, p. 24). However, for DFN conceptual models that incorporate more spatial organization (*e.g.* compound Poisson processes or fractal models), or even alternative fracture size distributions, this fortuitous result might not be obtained, and more realizations of each case might be necessary.

Surface/near-surface hydrological simulations tend to be less computationally demanding, depending on model complexity. A one-year period for a single catchment of the Laxemar subarea was solved in approximately 8 hours of computer time using MIKE SHE-MIKE 11, and significantly faster (6-14 minutes) using the simpler ECOFLOW model (Sokrut *et al.*, 2007).

4.3 Computational developments expected for next 5–10 years

Over the past two decades, continual order-of-magnitude improvements in central processing unit (CPU) technology have allowed model sizes and complexity to expand by orders of magnitude in terms of the number of degrees of freedom, while keeping simulation times within limits that are suitable for modelling project time scales. Advanced models are now routinely implemented and solved on desktop computers or workstations that are available on the ordinary commercial market (although the largest and most complex models have usually been implemented on more specialized computing platforms, up to the level of supercomputers).

For computers that are available through the ordinary commercial market, there has also been a consistent architecture defined by the Intel CPU series (386, 485, Pentium, *etc.*). For developers of hydrogeological models written in FORTRAN, C, or C++ languages, this situation has contributed to the widespread availability and competitiveness of standard compilers such as gcc (for Linux or UNIX platforms), which in turns has contributed to portability of these models. In this environment, it has been possible for multiple research groups and commercial companies to produce advanced modelling software with similar capabilities. This even includes non-proprietary open-source model software which permits collaborative development between institutions. From a regulatory perspective, this has meant that multiple alternative models are available, including some at very low cost, which can be used to check safety-case calculations.

A brief survey of computer science literature suggests that the period of continued rapid growth in CPU clock speed is reaching an end, due to fundamental physical limitations (excessive heat generation, power consumption and leaking voltage within semiconductor chips). The main direction of new developments is predicted to be toward multi-core processors, with the number of cores doubling with each processor generation (Buttari *et al.*, 2006). Specialized graphics processing units (GPUs) which outperform standard CPUs are also increasingly being used for high-performance numerical applications.

These developments point toward an increasingly heterogeneous computational environment for state-of-the-art hydrogeological models. Full exploitation of multicore processors will require parallel algorithms, but implementation of these algorithms may be complicated by divergent CPU (and/or GPU) designs. These divergent designs may require scientific programming software designed to exploit heterogeneous computing environments. One initiative in this direction is the Parallel Linear Algebra for Scalable Multi-Core Architectures (PLASMA) initiative, which is described at the ScaLAPACK project website (www.netlib.org/scalapack/).

The other major development that can be expected in the next 5-10 years is improved technology for distributed computing, or "cluster" computing. This gives increased possibility for parallel computations to be carried out on networks of ordinary computers linked by ethernets. Many methods for taking advantage of such interconnected systems have been proposed; the most widely known is the Linda programming environment, which involves just five statements added to normal sequential languages such as C, C++, or FORTRAN.

Hydrogeological models for site-scale modelling in crystalline hard rock are in many respects well suited to parallel algorithms. Mattson (1996) has described the following categories of algorithms that, in differing degrees, may be able to exploit these developments:

- Synchronous algorithms: tightly coupled manipulation of identical data elements, regular in space and time (*e.g.* finite difference computations for interior nodes, then updating with boundary information, usually in a time-stepping loop).
- Loosely synchronous algorithms: Tightly coupled but data elements not identical, irregular in space and time (*e.g.* adaptive finite-element grids).
- Asynchronous algorithms: unpredictable or nonexistent coupling between tasks, irregular in time and usually irregular in space (*e.g.* simulation and monitoring of complex systems

such as can arise with stochastic geometries and non-linear processes).

- "Embarrassingly parallel" algorithms (*e.g.* independent iterations, Monte Carlo simulations, distance computations, mesh generation, parallel genetic algorithms, simulated annealing, and other stochastic algorithms for calibration).

Areas in which parallel algorithms could be particularly effective for accelerating hydrogeological computations for crystalline hard rock include:

- computation of intersections and mesh generation for DFN models,
- calculation of finite-element matrices for large numbers of elements,
- vectorized calculations for iterative matrix solvers,
- simultaneous tracking of multiple particles for transport predictions

These possibilities can – and in some cases might already – be exploited by developers of state-of-the-art hydrogeological models. This will enable continued increases in the level of detail and representation of coupled processes for site-scale models of crystalline hard rock, over the coming 5 to 10 years.

However, exploitation of these possibilities may require specialized compilers, adapted for the architecture of each particular processor. This could increase costs for development of applications, and may also reduce portability, for example if a code is optimized for a particular supercomputer platform that the code vendor operates as a service to clients.

This raises a risk of a widening gap between proprietary models that are used by repository implementers, versus alternative, independent models that regulators will have access to. If the proprietary codes have limited portability, this may also impede efforts of regulators to make independent calculations using the implementers' models.

On the other hand, the increasing practicality of distributed computing may help to maintain a diverse and competitive set of models for site-scale hydrogeological modelling. Key areas to watch include developments in distributed programming environments (*e.g.* Linda) and numerical packages for heterogeneous/distributed computing environments (*e.g.* the PLASMA initiative). Dialogue between regulators and repository implementers may also help to promote standards for model developers, which will ensure portability and transferability of models for future regulatory compliance evaluations.

4.4 Expected limitations on datasets for model calibration

Availability of data to constrain heterogeneous models has been a key issue for application of increasingly sophisticated models. As summarized from the GEOTRAP workshops (NEA, 2002):

Models of groundwater flow are currently available that allow, in principle, a realistic representation of the structural variability of a geologic medium. Availability of data is the most important constraint on the use of these models. An effort still needs to be made, however, to improve our ability to incorporate a wide variety of different types of data (at length scales relevant for the system under consideration) in order to take full advantage of these models.

Over the past decade, significant advances have been made in terms of the amounts and types of data that can be brought into site-scale hydrogeological/hydrological models. Large datasets are now routinely incorporated to define:

- Topography (*e.g.* digital elevation models),
- Land cover (*e.g.* GIS models of regolith type and thickness),
- Time series data from hydrological monitoring (*e.g.* precipitation, potential evapotranspiration, and water levels in monitoring holes),
- Surface coordinates of inferred geological structures (*e.g.* lineaments on scales from kilometers down to decameters),
- Interpreted (hydrological) deformation-zone shapes based on interpolation/extrapolation from surface observations and borehole/tunnel intercepts.
- Fracture positions and orientations as mapped from tunnels or drillcore/borehole surveys, and
- Positions and shapes of underground openings (repository tunnels and shafts).

In addition, recent models have made use of:

- integrated interpretations of flowing features (*e.g.* Posiva Flow Log anomalies in combination with borehole mapping),
- hydrogeochemical interpretations (reference water proportions from sampling in drillholes),
- time-dependent responses during large-scale flow and tracer tests, and
- single-well injection-withdrawal tests

as key data for calibration and/or confirmation of models.

A very high density of additional flowing-feature data, in combination with fracture mapping data and related geophysical techniques, can expected to be obtained around tunnels during the repository construction phase. Indeed, improvements will be needed in methods for conditional simulation of DFN models, in order to make full use of these data.

However, for most of the rock volume that is considered in site-scale models, the amount of such data will likely remain near current levels. Drilling of additional deep holes to improve characterize site-scale heterogeneity is discouraged, due to concerns about compromising the bedrock's capacity to isolate the repository from the surface environment, as well as perceptions that the value of additional information obtained is low in relation to the cost of deep drillhole characterization.

Sparsity of high-quality hydrogeochemical datasets for model confirmation is perhaps the most serious constraint on emerging approaches to model confirmation. For sites such as Forsmark and Olkiluoto, the opportunity to obtain high-quality data from nominally undisturbed conditions is now past, due to extensive disturbance of these sites by drilling, pumping of groundwater, and (in the case of Olkiluoto) excavation of the ONKALO facility. Discrepancies in the locations of predicted vs. apparent depths for transitions in groundwater chemistry might be resolved by model refinements, but without additional data to check the models, these refinements might simply be regarded as fitting exercises.

Large-scale flow and tracer tests from boreholes are also likely to be limited in site-specific programmes that are moving on to the repository licensing and construction phase. However, repository construction can provide a valuable test of site-scale hydrogeological models, as demonstrated from prediction-and-evaluation exercises at the Äspö HRL, and similar ongoing work at ONKALO.

The limited time scale that is practical for large-scale hydrogeologic testing, and dissimilarity of the strongly converging flow fields during drawdown experiments in comparison with natural gradients, will be difficult to overcome with foreseeable new site-specific data. As concluded from the GEOTRAP workshops (NEA, 2002):

Calibration and testing over spatial and temporal scales that are relevant to performance assessment would, in principle, be the best method to build the confidence in models of flow and transport. Such calibration and testing is difficult to achieve, especially considering the very long travel times that are expected through the rock formations that are potentially acceptable to host a repository and the possible transient nature of the groundwater flow system. Analogues, both natural and anthropogenic, provide a possible means to address this difficulty.

Leaving aside the possibility to find suitable analogues, the inherent difficulties posed by differing spatial and especially temporal scales are likely to persist in data sets that can reasonably be obtained over the next decade.

4.5 What is sufficient based on the Finnish regulatory perspective?

The question of sufficiency of models is potentially a very broad one, from an academic research perspective. However, the Finnish regulatory framework for review is based on specific nuclear safety regulations including:

A: Nuclear Energy Act (990/1987)
D: Nuclear Energy Decree (161/1988)
GD: Government Decree on the safety of disposal of nuclear waste (736/2008)
YVL: STUK's Guide YVL D.5

These documents form the basis for a series of questions that can be applied to site-scale hydrogeological models to assess the sufficiency and expectations for the state of the art.

1. In order to analyze the release and transport of disposed radioactive substances, are the conceptual models appropriately drawn up to describe the physical phenomena and processes controlling the safety functions? [YVL E.5 704, A106]

Hydrogeological models based on the discrete-fracture network (DFN) concept are generally recognized as the most applicable approach for crystalline hard rock. The approach to deriving radionuclide transport parameters based on DFN models is supported by scientific consensus, *e.g.* as developed in the RETROCK project (European Commission report number EUR 21230 EN).

DFN models capable of representing coupled processes of nonreactive solute transport, heat transfer, and density-dependent flow, and to a lesser extent, hydromechanical and reactive transport, are now becoming available. Unsaturated-zone flow and infiltration processes are generally treated in a simplified fashion in site-scale hydrogeological models, although surface hydrological models can be used to justify these assumptions.

Site-scale applications still normally require simplifications for the sake of practicality, either in terms of upscaling methods or in terms of the range of physical processes that are represented. Where processes such as coupled density-dependent flow and transport are considered to be important (for example, long-term simulations of a coastal repository with changing coastline and surface conditions), upscaling from a DFN to a continuum porous-medium (CPM) is often used, sometimes referred to as equivalent CPM or ECPM models. This allows the use of well-established CPM codes that are capable of simulating these coupled processes.

The ECPM approximation is not necessarily valid for sparsely fractured bedrock. While equivalence has been demonstrated in some particular cases (Jackson *et al.*, 2001), this should be demonstrated for site-specific DFN conceptual models and parameters, as part of a safety case employing ECPM methods. Such a demonstration might be achievable by a small set of DFN realizations making use of justifiable simplifications (*e.g.*, neglecting density effects for the purpose of comparison), but it should not be neglected.

Conceptual models for DFN representation should also be examined and compared with reasonable alternatives, particularly with regard to statistical heterogeneity of the fracture population. This has rarely been done for DFN models used in site-scale models, but results from Geier (2011) show that the effect for flow to deposition holes could be significant. Conceptual as well as parametric uncertainties in the distributions of fracture size and transmissivity distributions are also important to check. Finally methods for deriving DFN models from site-investigation data frequently do not account for fracture channeling, except as a scaling factor when calculating effective transport parameters. The consequences of this approach should be addressed in the safety case.

2. Are the available models adequate to describe circumstances affecting the performance of safety functions? [YVL D.5 704, A106]

Hydrogeological models available today are adequate to describe most circumstances that are recognized as being significant for performance of safety functions. Two situations of concern, saline upconing and infiltration of dilute glacial meltwaters, have only been partly addressed by past quantitative modelling for Olkiluoto.

The first of these, saline upconing, could be addressed by using capabilities of models to model density-dependent flow due to salinity and thermal variations, in combination with a sufficiently detailed representation of the repository tunnels and its hydraulic interaction with the fracture network. Nested DFN-ECPM models and/or full-scale DFN models that represent the density-dependent flow phenomena provide two possible ways of addressing this deficiency. If ECPM models are used, they should be fully justified as discussed under the preceding question.

Capabilities for modelling infiltration of dilute glacial meltwaters have improved. However, methods for evaluating site-scale or regional-scale, coupled hydromechanical effects of the ice load on bedrock hydrogeology, are still limited. Also, understanding of periglacial and glacial conditions affecting recharge and discharge at the ground surface, and flow in the shallow bedrock, is still limited. The Greenland Analogue Project could be a source of data for developing and testing these aspects of site-scale hydrogeological model, over the next ten years.

3. Are the computational models appropriately derived from the respective conceptual models? [YVL D.5 704, A106]

The state-of-the-art computational models discussed in this report are derived by conventional numerical methods (finite element or finite difference). Most have undergone verification exercises which provide further assurance that the mathematical models are correctly implemented. One concern, particularly with proprietary commercial software, could be whether there is sufficiently transparent documentation for regulators to understand when non-physical modelling “tricks” are used to simplify or accelerate computations, or to account for additional coupled processes. These questions will need to be assessed on a case-by-case basis in safety case reviews. However, dialogue between regulators and implementers in advance of license applications can help to ensure that implementers, and their modelling consultants, give attention to this issue and develop appropriate documentation.

4. Are simplifications of the models and determination of the required input based on the principle that the performance of a safety function will not be overestimated while neither overly underestimated? [YVL D.5 704, A106]

Developers of state-of-the-art hydrogeological models tend to aim for increased realism with each successive version of their models. Thus they are not inherently conservative in the sense of ensuring that the performance of safety functions will not be overestimated (the first part of this regulatory question). This issue generally ends up as the responsibility of analysts who apply the models for specific calculations related to a safety case.

The model developers' aim for increased realism tends to promote the goal of ensuring that safety functions are not overly underestimated (the second part of this question). Availability of more realistic models, which can incorporate more detailed descriptions of spatially varying parameters, means that analysts will have less need to adopt overly conservative parameters that might be adopted for less refined models. Complex, relatively realistic models can also increase the value of simplified models that result from conservative argument, when the complex models are used to evaluate the degree of conservatism (NEA, 2002).

However, when analysts choose parameters for complex models, some pitfalls remain. For example, values of matrix diffusion parameters that are conservative in simple models for radionuclide transport might yield non-conservative models, if they are assumed during calibration of models based on palaeohydrological simulations to match hydrogeochemical data. Similarly, in DFN analysis, what is thought to be a conservative assumption about fracture size distributions might lead to non-conservative estimates of other DFN properties after calibrating to hydraulic data from boreholes. To avoid these pitfalls, conservative assumptions are best applied in later stages of modelling, after development of models which are as realistic as possible, and then only in calculation cases which are formulated so as to avoid unintended side effects.

6. Are the models and input data consistent with the scenarios, assessment period and disposal system? [GD §15; YVL D.5 A107]

Development of hydrogeological models for crystalline hard rock has, in large degree, been driven by consideration of scenarios, time periods, and disposal concepts for repositories in Fennoscandian and Canadian Shield environments. While applications to date have not always succeeded in meeting these goals (*e.g.* including density-dependent flow in realistic DFN representations), the current state-of-the-art models can handle most processes that are thought to be significant for the key scenarios and time scales. Methods for simulating features associated with the KBS-3 disposal system – including EDZ around tunnels and deposition holes, flow through backfilled tunnels, and criteria for deposition-hole emplacement – have also been demonstrated in various models, although not always combined in a single model.

Remaining weaknesses mainly concern the limited understanding – both in terms of conceptual models and data – for periglacial and glacial environments, which need to be considered for assessment periods on the order of 100,000 years.

7. Are stochastic models appropriately employed when the input data used in modelling involve random variations due to e.g. heterogeneity of rock? [GD §15; YVL D.5 A107]

State-of-the-art hydrogeologic models for crystalline hard rock have been developed that permit stochastic treatment of the system components where this is most relevant – including stochastic, discrete fractures in the bedrock and spatially varying properties within deformation zones. It should be expected that safety assessment calculations will make use of these capabilities, at least to the extent of demonstrating the significance of uncertainty that arises from hydraulic heterogeneity in the bedrock, and practical limitations on characterization of that heterogeneity.

With the most complex models that have been demonstrated, one risk is that the very sophistication of these models may limit assessment of uncertainties. One way for this to happen is when the computational demands of a complex model are so great, that this limits the number of stochastic realizations that can be evaluated. This situation appears to have occurred in several recent applications.

A second way is when a single site model is developed to such a level of sophistication, that alternative models may be discounted. The need to consider multiple alternative models applies to hydrologic models in general (Beven, 2001), and has also been pointed out within the regulatory context for a Swedish repository (Chapman *et al.*, 2010). The GEOTRAP workshops (NEA, 2002) also led to a conclusion that:

The widest range of models consistent with the available observations should be considered in order to evaluate conceptual model uncertainty (only a limited number of models may be selected from this range for further quantitative evaluations); the principle that alternative models should be considered applies not only to models of flow and transport, but also to underlying models such as those of geologic structure.

8. Are the uncertainties included in the safety analysis assessed by means of appropriate methods? [GD §15, YVL D.5 704, A108 (A105)]

The current state-of-the-art in hydrogeological models for crystalline hard rock permits quantitative analysis of uncertainties both by stochastic methods and by bounding analyses of key parameters. Thus capabilities exist for compliance with the Finnish regulation which calls for analysis of uncertainties by sensitivity analyses or probabilistic methods.

However, the sophistication of these models in terms of incorporating large data sets and heterogeneous parameters may also create difficulty in knowing if the analysis of uncertainties is complete. Methodologies for analysis of model sensitivities to large input-data sets and large parameter spaces may thus need to be a topic for future reviews.

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