Upscaling of Flow, Transport, and Stress-effects in Fractured Rock

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Abstract

One of many applications of geohydraulic modelling is assessing the suitability of a site to host a nuclear waste repository. This modelling task is complicated by scale-dependent heterogeneity and coupled thermo-hydro-mechanical (THM) processes. The objective here was to develop methods for (i) upscaling flow and transport in fractured media from detailed-scale data and (ii) accounting for THM-induced effects on regional-scale transport. An example field data set was used for demonstration.

A systematic framework was developed where equivalent properties of flow, transport, and stress-effects were estimated with discrete fracture network (DFN) modelling, at some block scale, and then transferred to a regional-scale stochastic continuum (SC) model. The selected block scale allowed a continuum approximation of flow, but not of transport. Instead, block-scale transport was quantified by transit time distributions and modelled with a particle random walk method at the regional scale.

An enhanced SC-upscaling approach was developed to reproduce the DFN flow results more simply. This required: (i) weighting of the input well-test data by their conductivity-dependent test volumes and (ii) conductivity-dependent correlation structure. Interestingly, the best-fitting correlation structure resembled the density function of DFN transmissivities.

Channelized transport, over distances exceeding the block scale, was modelled with a transport persistence length. A linear relationship was found between this persistence length and the macroscale dispersion coefficient, with a slope equal to a representative mean block-scale dispersion coefficient.

A method was also developed to combine well-test data and rock-mechanical data in estimating fracture transmissivities, and its application was demonstrated.

Finally, an overall sequential THM analysis was introduced allowing the estimation of the significance of waste-related thermo-mechanical (TM) effects on regional transport; here TM effects are calculated separately and their impact on fracture transmissivities were incorporated into the hybrid framework. For the particular case, their effects on regional-scale transport were small.

Keywords: Upscaling, fractured media, flow, solute transport, thermo-hydro-mechanical processes, hybrid approach, continuum approximation, discrete fracture network, stochastic continuum

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The contribution to the papers by the author is as follows:

I    Responsible for numerical method development, modelling, and most of result evaluation. The authors shared the conceptual model development and writing.

II   Responsible for numerical model development, modelling and most of result evaluation. The authors shared the conceptual model development and writing.

III  Responsible for numerical model development, modelling and evaluation and large part of the writing. Authors shared the conceptual model development.

IV   Responsible for numerical model development and modelling (except thermo-mechanical modelling) evaluation and most of the writing. Authors shared the conceptual model development.
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Abbreviations

1-D One-dimensional
2-D Two-dimensional
3-D Three-dimensional
EPM Equivalent Porous Medium
THM Thermo-Hydro-Mechanical
SC Stochastic Continuum
DFN Discrete Fracture Network
ADE Advective Dispersive Equation

Various scales were addressed in this thesis. For clarity, the following definitions are therefore made:

- regional scale: a kilometre-scale domain for which transport is to be solved.
- block scale: a cubic rock volume, with side length $\Delta x_{DFN}$, for which fracture network flow can be represented by conductivity tensors of equivalent porous media (i.e., it is the scale for valid “continuum approximation” of hydraulic flow).
- detailed scale: scale in which fracture network geometry and individual fractures that govern the transport properties of the medium are explicitly taken into account.
- support scale: the scale for which the heterogeneity in the SC approach is defined, such as the support scale of the underlying field measurements. It is often also equal to the scale of grid discretization in the SC models. Here it is denoted by the element size $\Delta x_{SC}$. 
1. Introduction

The understanding of flow and transport processes in fractured rock has improved considerably over the last decades [Wang (1991); NRC (1996); Tsang and Neretnieks (1998); Berkowitz (2002); Bodin et al. (2003)]. This progress has been driven by exploitation of natural resources, such as groundwater, petroleum reservoirs, and geothermal heat, but also rising environmental concerns regarding e.g. the mining industry and industrial toxic waste. A discipline that has greatly contributed to improving the understanding of fracture flow and transport is that of nuclear waste disposal.

The safe long-term disposal of high-level radioactive waste is a pressing issue for many countries that rely on nuclear power (WNA, 1999). The disposal of nuclear waste is a multifaceted subject involving politics, legislation, international treaties, engineering technology, public acceptance, but above all the decisive factor lies in the assurance of long-term safety.

A safety assessment is a complex matter in itself. It can be summarized as a detailed system description of the post-closure repository state, for which the consequences of potential future developments are evaluated with regard to long-term safety [e.g. SKB (1999); NEA (1997)]. The various considerations include both internal processes and/or external perturbations and a list of 134 generic Features, Events and Processes (FEPs) is considered relevant for safety evaluations by NEA (2000).

A performance assessment is more technical and limited to the processes relevant for the liability of the disposal system. Its purpose is to evaluate if a potential site meets the requirements in functionality for hosting a repository [Tsang et al. (1994); NEA (1997); Andersson et al. (2000)]. Such requirements are stipulated by legislation and regulation in terms of parameter ranges for specific suitability indicators (flow, transport resistance, etc.; Andersson et al., 2000). Here, geohydraulic modelling has a key role in providing predictions and uncertainty estimates of these [e.g. Hudson et al. (2001); Andersson et al. (2000); Rhén and Smellie (2003)].

The most fundamental requirement for a geohydraulic model is its ability to provide an adequate site-specific description (NRC, 1996). It is confronted by several difficulties, most notably due to the heterogeneity of the media, the large temporal and spatial scales, and the complex processes involved [Tsang et al. (1994); Tsang et al. (2000)]. This requires simplifications and innovative approaches. Therefore, performance assessments cannot rely on some standard “universal computer code”, but must integrate results
from several nested models, each being designed to target specific processes, scales, sites and/or scenarios (e.g., NEA, 2002). The assimilation of model results requires coherent treatment of modelling scales and particular consideration for different processes acting on different scales of time and space.

In this context, the upscaling of fracture properties is an important tool, arising from limitations in computer capacity. Here, two basic model representations of fractured rock are studied: the discrete fracture network (DFN) approach and the stochastic continuum (SC) approach. Both concepts entail benefits and disadvantages. The DFN model is superior at small scales as it accounts for the geometry and connectivity of the fracture network. The SC framework operates only with averaged equivalent properties of fractured rock and is therefore, owing to its parsimony, applicable to larger scales (Neuman, 1987). Its major drawback is that its simplified parameterization may be inadequate for fractured rock. Thus, DFN models can both be used to upscale detailed-scale data for use in large-scale SC models, and to evaluate the validity of doing so.

Geohydraulic modelling of fractured media is a multi-disciplinary science that requires combined insight in geology, rock mechanics, and hydrology. A geologic disposal system for nuclear waste is governed by the following coupled processes: thermal (T), hydrological (H), and mechanical (M) — collectively referred to as THM processes [e.g., Tsang, (1987); Tsang, (1991); SKB (1999)]. Coupling implies that the processes are dependent on each other through feed-back mechanisms (Jing et al., 1995). Therefore, models must consider all relevant aspects of THM-influence on the suitability indicators (e.g., flow and transport).

Confidence in such matters has for example been gained from international collaboration projects involving model-comparison exercises on limited amounts of in-situ data. This thesis is based on work conducted under participation in one such project (DECOVALEX III; Tsang et al., 2004). However, the findings made in this thesis are of a more general type and valid for the modelling and parameter estimation of fractured media in general. The application of these findings is therefore not confined to the field of nuclear waste disposal.
1.1 Objectives and aims

The overall objective of this thesis was to address two primary issues of geohydraulic modelling: upscaling of flow and transport in fractured media from detailed-scale data and accounting for thermo-mechanical-induced effects on regional-scale flow and transport. The specific aims were:

1. to compare the fracture network and stochastic continuum model principles in upscaling of hydraulic conductivity and to develop a new upscaling method based on the stochastic continuum concept (Paper I),
2. to develop an upscaling approach for solute transport to model regional-scale transport and to investigate the link between channelling and macro-scale dispersion (Paper II),
3. to develop a method to account for the stress regime in the estimation of fracture transmissivities from hydraulic borehole data (Paper III), and
4. to develop an overall approach to assess the importance of the thermo-mechanical effects on conductivity and regional-scale transport time in a hypothetical nuclear waste repository scenario, given a limited amount of site-specific, detailed-scale data (Paper IV).

In the following, first a general summary is given concerning the conceptual understanding and different modelling approaches presently available for fractured media (Section 2). Next, the general approach taken is described (Section 3), followed by the various sub-topics. These are upscaling of hydraulic conductivity at some support scale (Section 4) and exploring different strategies to upscale solute transport (Section 5). The results of these upscaling approaches are applied in a hybrid approach to solve regional transport (Section 6). Potential THM effects on hydraulic conductivity and regional-scale transport are examined (Section 7). Results are then summarized and discussed (Section 8). Finally, the conclusions drawn are listed (Section 9).
2. Background

2.1 Characterization of fractured media

A proper characterization of the highly heterogeneous fractured media is an important task for a number of environmental and engineering applications, such as the disposal of high level nuclear waste. Many countries plan deep underground storage for their nuclear waste. It is therefore crucial to obtain adequate data from potential sites, to evaluate their suitability for hosting a nuclear waste repository. Sweden is, after a survey of feasibility studies, now in the phase of site investigations. Two sites close to Åspö, Simpevarp and Laxemar (SKB, 2002a), and one site in Forsmark (SKB, 2002b) are currently under investigation to establish a foundation for deciding the site for deep storage. Thorough site investigations, performed during the last decades, also include: five sites in Finland, now focusing on one in Olkiluoto (Vaittinen et al., 2003), Yucca Mountain in US (Bodvarsson et al., 1999) and Sellafield, U.K (1989-1997; Holmes, 1997). An approved surface site investigation is ensued by construction of an underground rock characterization facility, to obtain three-dimensional data, such as the ONKALO facility under construction in Olkiluoto, the Exploratory Studies Facility in Yucca Mountain (ESF; completed in 1996) and the Rock Characterization Facility in Sellafield (RCF; rejected in 1997).

Confidence in predicting subsurface geohydraulic conditions from surface and borehole investigations has been gained from Underground Research Laboratories (URLs; NEA, 2001). The URLs, which also serve as “dress rehearsals” for future repository construction, facilitate in-situ experiments and supplementary rock characterization, which is indispensable for understanding processes in the repository environment. Major URL programmes have been undertaken during the last decades, including Stripa (Olsson et al., 1992) and Åspö hard rock laboratory (HRL; Rhén et al., 1997) in Sweden, Whiteshell URL in Canada, the Grimsel Test site (GTS) in Switzerland, the Fanay-Augères mine in France, and the Kamaishi and Tono mines in Japan.

Fractured rock is highly heterogeneous in comparison to porous media. Depending on the aperture of a fracture, its permeability can exceed that of the ambient rock matrix by many orders of magnitude. Therefore hydraulic flow in fractured media is mainly governed by the geometry and connec-
activity of its fracture network and by the individual fracture apertures. Thus, hydraulic data of fractured media typically displays strong variability in measurements at different locations depending on presence/absence of conducting and connected fractures.

2.2 Stochastic parameterization of data

A site investigation must minimize its detrimental influence on safety for future disposal at the site (Tsang et al., 1994). Thus, due to the destructive nature of borehole sampling, the data available for a site is typically scarce in relation to the domain that needs to be characterized (Berkowitz, 2002), which causes a source of uncertainty. It is however important to distinguish between variability and uncertainty: a quantified property may exhibit spatial or temporal variability, although properly defined for given space-time points, while uncertainty reflects incomplete characterization in space and/or time (NEA, 1997). This necessitates the use of a stochastic framework to estimate the range of possible outcomes for a process that depends on an incompletely characterized and spatially variable property.

There are two fundamentally different concepts to transfer data to models: deterministic and stochastic parameterization (Niemi, 1994). Deterministic parameterization is the traditional approach to model porous media where heterogeneity generally is low. Here, the model features are assumed to be known, and applied directly as recorded at point measurements and smoothly interpolated for uncharacterized surroundings. However, the strong heterogeneity of fractured media in combination with the inevitably incomplete site characterization often makes a deterministic approach inadequate. The reason is that smooth interpolation neglects point-wise variability in data, and hence fails to reflect the variability and uncertainty of a model (Deutsch and Journel, 1998).

A stochastic description treats a property as a random variable and its observed values at various points as realizations of a random process [Gelhar (1993); Kitanidis (1997); Niemi (1994); Deutsch and Journel (1998); Mishra, (2002)]. A data set provides an estimate of the property ensemble that defines the possible outcomes of the random variable at any given point in space. Stochastic modelling then treats multiple realizations of the random variable to estimate the range of possible outcomes for a process that depends on the medium property. The stochastic principle can be used to parameterize both the discrete fracture network and stochastic continuum models. However, it is also a question of scale. In practice, well-defined large features, such as regional fault zones, etc., can be treated deterministically in models, while smaller features, or background conductivity, are stochastically described [e.g., Rhén et al. (1997); Selroos et al. (2002)].
2.3 Modelling representation of fractured media

The two principal model representations for fractured media considered in this thesis are discrete fracture network (DFN) modelling [e.g., NRC (1996); Dershowitz et al. (1998)] and the stochastic continuum (SC) concept (Neuman, 1987). These alternative concepts entail both benefits and limitations. Hence, often the greatest advantage of the two concepts can be gained in a combined usage, often referred to as “hybrid approaches” [Berkowitz (2002); NRC (1996); Jackson et al. (2000); Svensson (2001a-b); Min (2003); Schwartz and Smith (1988); Benke and Painter (2003); Papers I, II and IV]. In a hybrid approach the two concepts are used complementary.

2.3.1 Discrete fracture network modelling

The fracture network concept is considered the most realistic representation of fracture flow, as it accounts for individual fracture geometry and connectivity of the network. However, the spatial configuration of a fracture network (mainly connectivity and clustering) is often difficult to parameterize (NRC, 1996). Fracture network data are generally compiled from 1-D and 2-D geologic observations (e.g., boreholes and trace maps). To parameterize its underlying true 3-D fracture network, these data need to be extrapolated into the third dimension [Dershowitz and Herda (1992); La Pointe (2002); Barton (1995); Pigott (1997)]. Additionally, the hydraulically active fracture network is not equal to the geologically observable fracture network, as not all fractures are connected and conductive.

Fracture network properties can be scale-independent or exhibit fractal scaling, i.e., self-similarity at various scales [e.g., Odling (1997); Bour and Davy (1999); Darcel et al. (2003)]. A variety of conceptual models have been developed for the generation of numerical fracture networks. These include e.g., Poisson Plane, Baecher, Nearest Neighbour, War Zone, and several fractal models [NRC (1996); Dershowitz et al. (1998)]. Statistical analyses of geologic and hydraulic data provide means to select the most appropriate model for a particular site. The BART Baecher model [Baecher et al. (1977); Dershowitz et al. (1998)] is commonly used [e.g., Outters and Shuttle (2000); Cvetkovic et al. (2004)].

The computational demand of a DFN model often restricts its usage to smaller scales which necessitates other more parsimonious methods at larger scales, e.g., models based on the stochastic continuum concept. Nevertheless, DFN models are irreplaceable conceptual tools to model the influences that a fracture network has on processes at smaller scales.

In this thesis, the DFN model was used to evaluate the validity of the SC approach and to upscale detailed-scale data as input to a regional-scale SC model. It was also used to quantify the potential impact of stress regime on the estimation of fracture transmissivity from borehole data, and thermo-
mechanical influence on flow in the repository near-field. The hydraulic parameterization of a DFN is discussed below.

2.3.2 Stochastic continuum modelling

The stochastic continuum approach assumes that, above a certain scale a fractured medium behaves as a continuum. It operates with volume-averaged properties for discretized volumes of a fractured rock. The volumetric properties used must be equivalent to the properties of the fracture network within each volume. For its application, the influences of heterogeneous details must average out within the rock volume, such that the medium behaves as a homogeneous medium at some scale. In other words, the approach relies on the dissipative nature of flow that tends to level out the effects of heterogeneity over a volume (Vogel and Roth, 2003). Consequently, the approach addresses heterogeneity at scales larger than that of the continuum approximation, but is generally unable to resolve any heterogeneity below that scale (Rubin et al., 2003).

The range of possible outcomes of a process (expectation and uncertainty) can be analysed in a stochastic framework, providing that such equivalent properties can properly be defined at some scale. This is often done by modelling a process in multiple random property fields that each honour experimental statistics. Random fields or realizations are equally possible versions of the spatial configuration for a property. They can be either unconditional or conditioned to measured data at locations of the measurements (e.g., Niemi, 1994). In the latter case they are often generated by kriging [e.g., Gelhar (1993); Kitanidis (1997)]. Kriging is the best linear unbiased estimate to statistically honour field data in terms of in expected parameter values, parameter variability and spatial correlation (Deutsch and Journel, 1998). For example, the uncertainty in a flow field, arising from incompletely characterized conductivity, can be estimated by analyzing the results of a large number of flow simulations from multiple stochastic conductivity realizations [Gomez-Hernandez and Gorelick (1989); Niemi (1994)].

2.4 Hydraulic data parameterization

The validity of geohydraulic models relies on their ability to reflect hydraulic system of the medium. Hydrological model parameters are often derived from various types of in-situ hydraulic borehole tests (NRC, 1996). The interpretation and application of hydraulic data is the most critical, yet the most uncertain, step in geohydraulic modelling especially in cases of strongly heterogeneous fractured media. Test results are typically converted into apparent conductivity values which are only inferred medium properties, not actual quantities of the medium (Follin and Thunvik, 1994). Linking
the test results to the actual hydraulic characteristics of the “sampled rock volume” or “extent of a fracture network” is not straightforward [NRC (1996); Berkowitz (2002)]. One reflection of this is that hydraulic data of fractured media are found to depend on the scale of measurement [Clauser (1992); Follin and Thunvik (1994); Niemi (1994)], as discussed below.

A specific feature of conductivity in fractured media is its dependence on stress. This has been observed, both in terms of depth trends [e.g., Hudson and Harrison (1997); Carlsson and Olsson (1977); Ahlbom and Smellie (1991)] and in terms of conductivity anisotropy [e.g., Rutqvist and Stephansson (2003); Barton et al. (1995); Carlsson and Olsson (1979); Talbot and Sirat (2001); Rhén et al. (1997)]. Additionally, hydraulic tests are particularly sensitive to properties in the vicinity of the borehole. These properties are subject to change owing to the drilling of the borehole, i.e., “skin-effect” (Bidaux and Tsang, 1991), and the pressure of the hydraulic tests (Rutqvist, 1996).

2.4.1 Input for fracture network models
Fracture transmissivity is governed by its aperture, i.e., the separation distance between its two bounding rock surfaces [e.g., Bear (1993); Hakami (1995)]. The aperture of a fracture is spatially variable with complex geometrical configuration [Hakami (1995); Lanaro (2001)]. Furthermore, detailed information concerning apertures is rarely available in practical cases (Berkowitz, 2002). Fracture transmissivity is highly sensitive to its aperture, and therefore the apertures visible in boreholes are too unreliable for modeling purposes. Instead, DFN models often employ different types of “equivalent apertures” to describe the process of interest (Tsang, 1992). The equivalent hydraulic aperture refers to the opening between two parallel plates with equivalent transmissivity to the real, rough-walled fracture [Zimmerman et al. (1992); Bear (1993); Zimmerman and Bodvarsson (1996a)]. The so-called cubic law is used to relate the hydraulic aperture, $b$, to the transmissivity, $T$, of a fracture with unit width

$$ T = \frac{\rho g b^3}{12 \mu}, \quad (1) $$

where $\rho$ and $\mu$ are density and dynamic viscosity of water, and $g$ is gravitational acceleration.

As the hydraulic aperture is only an equivalent parameter for fracture bulk-flow, its relation to solute transport [Silliman (1989); Dverstorp et al. (1992); Tsang (1992); Cvetkovic et al. (2004)] and mechanical deformation [Rutqvist (1995); Corneta et al., (2003); Olsson and Barton (2001); Rutqvist and Stephansson (2003)] in a fracture is not obvious. The dispersion of sol-
ute transport in a fracture depends on solute diffusion into stagnant water and channelled flow paths arising from the roughness of fracture walls [Moreno et al. (1990); Tsang (1993)]. The mechanical deformation of a fracture depends on the contact area between the asperities of the opposing fracture surfaces and is therefore also linked to the roughness of fracture walls (Hakami, 1995). As neither of these processes directly relate to the bulk-flow of a uniform fracture, the concepts of equivalent “mechanical,” respectively, “transport” apertures are also used.

The proper hydraulic parameterization of a DFN model obviously requires that hydraulic well-test data are honoured. This can be calibrated by simulating “numerical well-tests” [Cacas et al. (1990a); Niemi et al. (2000)]. In other words, stochastic transmissivity is assigned to fractures based on some initial estimate and “borehole tests” are simulated, and iteratively updating the transmissivities until simulations are in agreement with hydraulic data.

However, iterative flow simulations are time-consuming and therefore a simpler probabilistic method can also be used to estimate fracture transmissivity [Osnes et al. (1988); Osnes (1989)]. The method searches for the fracture transmissivity distribution that is statistically most likely to reproduce the borehole data. The method assumes that the net transmissivity of a tested borehole interval, $T_i$, equals the summed transmissivities of all conductive fractures, $T_{ij}$, that intersect an interval $i$.

$$T_i = \sum_{j=1}^{n_i} T_{ij}; \quad \log T_{ij} \sim N(\mu_{\log T}, \sigma_{\log T}),$$

where $T_i$ is the measured transmissivity of the interval $i$, $n_i$ is the number of conductive fractures that intersect the interval $i$, and $T_{ij}$ is the transmissivity of the $j$th conductive fracture within $i$. Fracture transmissivity is often assumed to be log-normally distributed (defined by mean and standard deviation of log-transformed transmissivity, $\mu_{\log T}$, respectively, $\sigma_{\log T}$).

In using this approach, the parameters are not entirely independent, i.e., an interval transmissivity can be explained, either by many low-transmissive fractures, or by few high-transmissive fractures. Hence the method does not guarantee a unique result, but rather a range of equally probable results [Niemi et al. (2000); Paper I]. This method has also been further developed for variable aperture and interconnected fractures (Dershowitz et al., 1998). However, it does not account for potential effects of the in situ-stress regime, as discussed above and will be analyzed in more detail (Paper III).
2.4.2 Input for stochastic continuum models

The continuum approximation is the core of the SC approach, and therefore its application to fractured rock cannot be taken for granted. Hydraulic characterization of fractured media is often evaluated in the form of equivalent conductivities for sealed borehole sections, i.e., assumed volume-averaged quantities. It is therefore tempting to treat such data as EPM properties in a SC approach, as is often done for porous media. Neuman (1987) was the first author to propose applying this approach for fractured media by assuming that the scale of hydraulic data (defined as the sealed borehole interval of measurements) can be directly used as the support scale of the SC models. However, while such a direct approach often is practical, it does involve two ambiguities: (i) the data actually relates to an undefined rock volume (Paper I) and (ii) the continuum approximation for this uncertain volume is generally unfounded.

The validity of the SC modelling approach requires that the medium indeed exhibits continuum behaviour at the support scale used. This can be examined by means of DFN flow simulations (Section 2.5.3). Depending on the nature of a fractured medium, the DFN flow simulations can derive EPM properties at some valid support-scale, which can then be consistently used as input in an SC model. This procedure of combining the DFN and SC modelling principles is referred to as a hybrid approach.

2.5 Upscaling fractured media properties to a continuum approximation

Upscaling procedures are used when the achievable spatial resolution in numerical models is coarser than the scale of measured heterogeneity (Wen and Gomez-Hernandez, 1996). Upscaling has been defined as: “means by which appropriate parameter values, processes and conceptual models are assigned to the larger scale of performance assessment or process-level models” (SNL, 1999). In other words, detailed-scale data are used to derive equivalent properties at a coarser scale for application in large-scale models. Under certain criteria, a medium property can approximately be represented by a coefficient of an Equivalent Porous Medium (EPM; NRC, 1996). For example, the flow behaviour in a given rock volume may be approximately described by a volume-averaged conductivity, that corresponds to an equally permeable continuum-type medium. This analogy is known as continuum approximation and is frequently used both in geohydraulic modelling and field experiments.

Thus, property upscaling entails a homogenization of the medium where the impact of small-scale heterogeneity on a process must average out, or “dissipate” (Vogel and Roth, 2003). Strictly speaking, equivalent properties
imply that the exclusion of fine-scale details must not affect the end result of the processes studied. In practise, however, upscaling is a compromise between constraints in computational capacity and precision; in all upscaling techniques fine-scale details are lost, which eliminates complete equivalence between use of detailed-scale and upscaled properties (Tsang et al., 1994). Methods have therefore been developed to compensate for wiped-out heterogeneity effects at subgrid-scale (e.g., Rubin et al., 2003).

However, the homogenisation of a medium is not always attainable, e.g. in cases where a medium displays certain types of multi-scale heterogeneity [e.g., Odling (1997); Le Borgne et al. (2004)]. It has been shown that multi-scale heterogeneity can be expected for fracture networks that exhibit particular fractal relationships in the spatial distribution of fractures [Bour and Davy (1999); Darcel et al. (2003)], their fracture length distribution [Odling (1997); Bour and Davy (1998)], and/or in aperture correlation to fracture lengths (de Dreuzy et al., 2002). However, as a practical modelling tool some authors do employ continuum approximation at some support scale, even for fractal media (e.g., Liu et al., 2004).

2.5.1 Scale dependency in conductivity

The conductivity of fractured rock defined over a volume is generally scale-dependent (NRC, 1996). Compiled laboratory and field experiments in crystalline rock indicate increasing geometric mean and decreasing variance in conductivity for increasing scales of measurement [Clauser (1992); Follin and Thunvik (1994); Vidstrand (1999); Rhén et al. (1997)]. Unless a medium displays fractal behaviour, this reduction in variability with larger measurement-scales is well-explained, as it involves averaging over larger volumes. The scale effect in mean conductivity, on the other hand, is less obvious; it can not be justified in the general case, partly because it depends on the dimension of flow, eq. (3).

The subject has been well-studied in the context of porous media, often under idealized assumptions, such as moderate heterogeneity, isotropic correlation, statistical homogeneity, infinite domain, log-normal conductivity, i.e., criteria not necessarily fulfilled in fractured media. The term effective conductivity, \( K_{\text{eff}} \), is often used to represent the average flow in a heterogeneous medium. Perturbation methods applied for stochastic differential equations provide an approximate \( K_{\text{eff}} \) as a function of support-scale variability and flow dimension for a moderately heterogeneous medium (e.g., Gelhar, 1993)

\[
K_{\text{eff}} = K_s \exp \left[ \frac{1}{2} - \frac{1}{D} \sigma_{i,k}^2 \right] ; \quad D = 1, 2, \ or \ 3 ,
\] (3)
where $K_g$ and $\sigma_{\ln K}$ are the geometric mean and standard deviation of logarithmic conductivity at some support scale and $D$ is dimensionality of the flow system. According to eq. (3), heterogeneity enhances 3-D flow (i.e., $K_{\text{eff}}$ increases with increasing $\sigma_{\ln K}$), has no impact on 2-D flow and reduces 1-D flow. Furthermore, eq. (3) implies that the effective conductivity of a given 3-D domain, may be characterized by small-scale measurements with high variability and low geometric mean, or large-scale data with lower variability and higher geometric mean, which agrees with most field observations [e.g., Clauser (1992); Rhén et al. (1997)].

However, many criteria for eq. (3), especially low heterogeneity ($\sigma_{\ln K} < 1$), are rarely fulfilled for fractured rock. Margolin et al. (1998) used percolation theory to derive a generalized scaling between support-scale conductivity, effective conductivity, and fracture network properties. Their relationship is rather similar to eq. (3), but is less sensitive to heterogeneity. Furthermore, there are also observations where 2-D flow displays increasing conductivity with support-scale (Sánchez-Vila et al., 1996). This discrepancy cannot be captured by normal SC models that assume log-normal conductivity with its spatial correlation defined by a single variogram (Sánchez-Vila et al., 1996). Supported by geological observations, indicator simulations (Deutsch and Journel, 1998) with higher correlation for high conductivity than for the remaining background conductivity, proved useful to explain these observations (Sánchez-Vila et al., 1996). It has also been demonstrated that effective conductivity can exhibit unlimited increase with support-scale for fractal 2-D fracture networks with apertures correlated to fracture length (de Dreuzy et al., 2002).

On the other hand, Hunt (2003) demonstrated with percolation theory that 3-D block conductivity can decrease with size of the averaging domain. The author studied highly heterogeneous media in a 3-D domain with side-length exceeding the characteristic distance between flow paths. Such critical path analyses are generally considered more appropriate than the SC description for highly heterogeneous fractured media [Wang (1991); Bour and Davy (1998)].

These contradictory findings raise concerns both regarding the reliability in field observations and their application in the SC framework. For example, the observed scale effect in mean block conductivity may be caused by inadequate sampling or inappropriate inference from data [Clauser (1992); Follin and Thunvik (1994); NRC (1996); Hunt (2003)]. These concerns emphasize the difficulty in modelling highly heterogeneous fractured rock consistently over a variety of scales.

2.5.2 Methods based on equivalent porous media

The upscaling of conductivity for moderately heterogeneous porous media is relatively well-established [Wen and Gomez-Hernandez, (1996); Renard and
The main reason is that for porous media, even small-scale hydraulic data can generally be assumed to satisfy continuum behaviour. Some porous-media based upscaling methods are also applied for fractured media, under the assumption that borehole data fulfil the criteria of EPM.

Walker et al. (2005) compared an empirical upscaling (based on compiled field data by Rhén et al., 1997) to upscaling with eq. (3). Several upscaling techniques are based on generating conductivity fields at measurement-scale, and calculating upscaled conductivity from blocks which contain multiple measurement values. These include upscaling calculations based on e.g. local averaging methods or Laplacian flow solutions. Local averaging techniques assume that measurement-scale conductivity can be upscaled without flow simulations [e.g. Pozdniakov and Tsang (1999); Vidstrand (2001); Maschio and Schiozer (2003)]. Instead, they are based on generalized relationships and are therefore simple and fast procedures. The Laplacian solutions depend not only on conductivity measurements, but also on the flow conditions within and around the block to be upscaled [e.g., Tran (1996); Chen et al. (2003)] i.e., they also consider the connectivity between blocks. Paper I explores how an EPM-based upscaling method can be derived from fracture network-based upscaling.

2.5.3 Fracture-network based upscaling methods

DFN-based upscaling can be considered the most reliable method to derive EPM properties of fractured media. The reason is that this method allows the validity of the continuum approximation to be evaluated. However, the validation is based on flow simulations of the fracture network and is therefore not infallible, as it provides that the DFN model indeed reflects the medium studied.

Direct methods have been suggested that estimate EPM properties from fracture data without flow solutions [Oda (1986); Svensson (2001a-b)]. In these methods, the block-scale conductivity is approximated by superimposing the transmissivities of all individual fractures that intersect a rock volume. Similarly to the local averaging techniques (previous section), these methods do not consider connectivity of the fracture network (c.f. Jackson et al., 2000). Zimmerman and Bodvarsson (1996b) suggested another direct numeric procedure to sequentially reduce a fracture network into an orthogonal grid where fracture transmissivities are replaced by an approximately equivalent value. Nevertheless, to confirm the validity for a continuum approximation at some scale, flow simulations are required.

The classical upscaling of fracture networks [e.g., Long et al. (1982); Cascas et al. (1990a)] is based on flow simulations where the equivalent conductivity is determined at some scale, in multiple directions. For example, in 2-D upscaling with no-flow boundary conditions parallel to the gradient, direc-
tional conductivity $K(\theta)$ can be determined by means of flow simulations for a fracture network subject to a gradually rotated hydraulic gradient

$$Q(\theta) = -\frac{\Delta h}{\Delta x} A K(\theta),$$  \hspace{1cm} (4)

where $Q(\theta)$ is the flow in direction $\theta$, $A$ the cross sectional area to the flow and $\Delta h/\Delta x$ is the imposed gradient. The fractured medium is of continuum-type if the obtained directional conductivities follow the transformation of a second order symmetric tensor (Harrison and Hudson, 2000). The hydraulic conductivity $K_{EPM}(\theta)$ of an anisotropic porous medium can be calculated from its tensor for any direction $\theta$,

$$K_{EPM}(\theta) = K_1 \cos^2(\theta + \xi) + K_2 \sin^2(\theta + \xi),$$  \hspace{1cm} (5)

where $K_1$ is the major and $K_2$ is the minor principal conductivity and $\xi$ is the direction of major principal conductivity. Here, the angle $\theta$ is counterclockwise, while $\xi$ is clockwise from the horizontal, such that $K_{EPM}(\xi) = K_1$.

A practical method to confirm if directional conductivity follows a tensorial transformation is to examine if a radial plot of $K_{EPM}(\theta)^{\frac{1}{2}}$ versus its direction $\theta$ follows an ellipse (Long et al., 1982). The larger the deviation from an ellipse, the worse is the continuum approximation for the network studied. In its 3-D extension, a spherical plot of $K_{EPM}(\theta,\phi)^{\frac{1}{2}}$, must resemble an ellipsoid (Niemi et al., 2000). For a statistically homogenous medium, the possibility for a valid continuum approximation enhances with larger scale of averaging, high fracture density, mixed fracture orientations and low variability in fracture aperture (Long et al., 1982).

The upscaling of a stochastically parameterized fractured medium requires the above described procedure to be repeated for multiple realizations. In case the continuum approximation is found valid, upscaled conductivity may also display variability and in turn provide stochastic input for the SC approach. To avoid immense numerical calculations, Hudson and La Pointe (1980) described a practical approach to use the electric analogue of hydraulic conductivity in fracture network-based upscaling. Their approach was to construct an electric circuit replica of the fracture network and to calculate its equivalent hydraulic conductivity at various points and in different directions from electric measurements. Upscaling procedures have also been developed to account for the stress regime [Zhang et al. (1996); Zhang and Sanderson (1999); Min et al. (2004b)]. These methods are, however, not conditioned to hydraulic data. A method to account for the stress regime in upscaled conductivity is suggested in Paper III.
2.6 Transport in fractured media

Transport in fractured media is governed by different mechanisms at various scales [Wang (1991); Moreno et al. (1997); Bodin et al. (2003)]. In fractured rock, the solute transport takes place along highly channelized flow paths [Abelin et al. (1991); Tsang (1993); Tsang and Neretnieks (1998)]. This channelling effect arises from the fact that flow tends to seek the path of least resistance [Tsang and Tsang (1989); Moreno and Tsang (1994)]. The channelling phenomena are found both at the fracture-network scale and at the fracture scale, i.e., arising from the non-uniform aperture within a fracture plane. The variable advective velocities of these flow paths result in longitudinal spreading of a solute at macro-scale [Neretnieks (1983); Moreno et al. (1997); Bodin et al. (2003); Bruderer and Barnabe (2001)].

At the temporal and spatial scales associated with disposal of nuclear waste, matrix diffusion is probably the most important retardation mechanism [Neretnieks (2004); Moreno et al. (1997)]. The diffusion facilitates the exchange of solute between fast and slow flow paths and also into the pores of the rock matrix [Neretnieks (1993); Cvetkovic et al. (1999); Andersson et al. (2004)]. The stagnant water volume of the rock matrix and its area available for sorption are orders of magnitude higher than those of fractures (Cvetkovic et al., 1999). Thus, matrix diffusion has a dominating effect on macro-scale dispersion. However, a consequence of channelling in the fracture plane is that solute is only exposed to a fraction of the total fracture area (e.g., Abelin et al., 1991). Therefore, two of the most critical parameters for reactive transport in fracture rock are considered to be transit time, \( \tau \), and transport resistance, \( \beta \) (Cvetkovic, 1999). For a parallel plate fracture, \( \beta \) is the ratio between the exposed fracture area and the volumetric flow rate of a uniform channel [m\(^2\)/(m\(^3\)/s)] which is equal to the “flow-wetted surface” (Moreno and Neretnieks, 1993) or the “specific wetted area” [e.g., Moreno et al. (1997); Dverstorp et al. (1992)].

A compilation of field experiments indicate that macro-scale dispersion increases with travel distance (Gelhar et al., 1992). Analytical solutions of the ADE are often used to analyze the dispersion of experimental tracer breakthrough curves (Bodin et al., 2003). However, tracer experiments in fractured rock typically reveal “anomalous” breakthrough curves (non-Fickian type) that are characterized by early initial arrival and particularly long tails [Tsang and Neretnieks (1998); Kosakowski (2004); Becker and Shapiro (2000); Shapiro (2001); Andersson et al. (2004)]. It is difficult to fully resolve whether these anomalies result from the variable advective velocity of different flow paths (Shapiro 2001) and/or diffusive mass transfer between flow paths and either stagnant water or rock matrix (Andersson et al., 2004).

In terms of modelling, the channelized transport arising from non-uniform apertures within a fracture plane can be modelled by assuming the cubic law

\[ k(x) = k_0 (1 + b x^k) \]

where \( k(x) \) is the permeability as a function of position along the fracture, \( k_0 \) is the permeability at the origin, \( b \) is a parameter that controls the rate of decrease of permeability, and \( k \) is an exponent that determines the shape of the permeability profile. This model is useful for describing the reduction of permeability due to the presence of fractures in a rock matrix.
to be valid locally [Moreno et al. (1990); Tsang (1993); Xu et al. (2001); Cvetkovic (1999)]. However, many DFN models use uniform hydraulic apertures to solve the bulk-flow in fractures (Section 2.4.1) which does not resolve the channelized flow (Berkowitz, 2002). Therefore, Nordqvist et al. (1992) demonstrated an approach to transfer the dispersion observed in individual fractures with non-uniform aperture distributions onto the flow field of a fracture network with uniform hydraulic apertures. DFN models have also been developed to account for the limited flow-wetted surface of fracture channels [Cacas et al. (1990a-b); Dverstorp et al. (1992); Moreno and Neretnieks (1993); Outters and Shuttle (2000)].

Solute dispersion is more sensitive to heterogeneity of the medium than is flow, and is therefore also less likely to exhibit continuum-type behaviour [e.g., Endo et al. (1984); Cacas et al. (1990b); Xu et al. (2001)]. Because of the difficulties in using continuum models for transport, on the one hand, and the computational limitations of DFN models, on the other, innovative methods are needed for regional-scale problems [NRC (1996); Berkowitz (2002)]. Many recent approaches rely on various forms of stochastic Lagrangian parameterization to transfer particle motion from “subdomain” DFNs to the regional scale [e.g., Schwartz and Smith (1988); Scher et al. (2002); Parney and Smith (1995); Benke and Painter (2003)]. Typically, stochastic particle motion is learnt from particle tracking in “subdomain” DFNs and then applied in terms of a random walk at the regional scale.

2.7 Progress in modelling of fractured media

Over the last decades, international collaboration projects have contributed much in improving the confidence of geohydraulic modelling. These have been forums for model-comparisons, exchange of data, process conceptualizations, multi-disciplinary expertise and mutual peer review. On initiative from the Swedish Nuclear Power Inspectorate (SKI) in 1981, a series of international collaboration projects started within the OECD Nuclear Energy Agency (NEA); International Nuclide Transport Code Intercomparison study (INTRACOIN), Hydrologic Code Intercomparison Study (HYDROCOIN; SKI/NEA, 1992), International Transport Validation Study (INTRAVAL; SKI/NEA, 1997) and Project on Radionuclide Migration in Geologic, Heterogeneous Media (GEOTRAP; NEA, 2002). The main objective has been confidence-building in the role of numerical modelling as a tool for performance assessments by inter-code accuracy verification and model validations against in-situ experiments and further advancing the understanding of chemical and physical processes of importance for performance assessments (Larsson, 1992).

Another extensive project on improving prediction ability for solute transport in a geological repository setting is the Tracer Retention Under-
standing Experiment (TRUE), which was managed during the last decade by the Swedish Nuclear Fuel and Waste Management (SKB). At the Äspö HRL, in-situ tracer experiments with sorbing solutes were conducted at repository depth for well-characterized flow paths with scales ranging between 10 and 100 m. With the objective to assess the retention mechanisms that link hydraulic flow to solute transport, results were interpreted using a variety of conceptual models; their major difference being parameterization of heterogeneity (Poteri et al., 2002).

The DECOVALEX project (DEvelopment of COupled models and their VALidation against EXperiments in nuclear waste isolation) was initiated 1992 to improve the understanding and model-descriptions of coupled THM processes at various scales, which are of relevance for performance assessments [Jing et al. (1995); Hudson et al. (2001); Tsang et al. (2004)]. A primary concern of the third phase was to examine the relevance of considering THM-coupled modelling in the framework of performance assessments and to assess its impact (Hudson et al., 2001). As part of this third phase, a benchmark test was formulated to explore the impact of TM changes on the repository near-field in terms of regional-scale transport, with a special emphasis on the associated upscaling. A limited data set from the Sellafield site was made available to different research teams (Andersson and Knight, 2000). Their task was then to develop parallel approaches to upscale the data and assess the potential influences that a hypothetical repository emplacement and its thermal emission may have on regional-scale transit time. Results of the various approaches were then compared to quantify the relevance of such THM effects, in relation to the uncertainty arising from the limited data set (Andersson et al., 2003). This thesis is based on findings made during the participation in this project.
3. Approach

This thesis explores an overall strategy: (i) to model regional-scale flow and transport in a fractured rock site, given a limited amount of geologic and hydraulic data, and (ii) to account for the thermo-hydro-mechanical (THM) effects of a nuclear waste repository on the transport. The research has been conducted through participation in an international collaboration project focusing on coupled THM processes in fractured rock (DECOVALEX III; Tsang et al., 2004). The particular task undertaken was to analyze the regional-scale transport and the role of the related THM effects in a hypothetical scenario related to deep disposal of high-level nuclear waste (Andersson and Knight, 2000), and to develop methods for upscaling the relevant model parameters. The model scenario is based on field data from Sellafield, England. Sellafield is a fractured rock site that has been intensively investigated by Nirex (e.g., Nirex, 1997a-d) in connection with nuclear waste. The database used is incomplete and not intended to reflect the characteristics of this particular site, but was used merely as an example of a realistic fractured rock database.

In particular, the task given was to assess the THM-effects on two critical parameters for transport in fractured rock (Cvetkovic, 1999), namely transit time, \( \tau \),

\[
\tau(s) = \frac{\int_0^s ds}{v(s)},
\]

and transport resistance, \( \beta \)

\[
\beta(s) = \frac{\int_0^s \frac{ds}{v(s) b(s)}}{2}.
\]

where \( v \) and \( b \) are spatially varying fluid velocity and aperture, respectively, at a trajectory distance \( s \) from the release point.

A hybrid approach incorporating the use of DFN modelling at the local scale to a SC model at the large scale was pursued as the main approach. The first step was hence to explore the possibility to approximate flow and trans-
port by means of continuum properties at some block scale $\Delta x^{DFN}$. This scale must be large enough to include a sufficient amount of fractures for continuum approximation to be valid, yet small enough to be handled by a DFN model. The results indicate that for the present data continuum representation is possible for flow (Paper I), but not for transport (Paper II), at least not at the same support scale. Therefore a new method was developed for up-scaling and modelling regional-scale transport for such data (Paper II). The method developed also provides means to explore the relationship between channelized transport and macro-scale dispersion.

In the overall approach taken, the DFN model has a central role in transferring detailed-scale data to the regional-scale model and in verifying the validity of the SC approach at the support scale of the regional-scale model. However, the hydraulic properties of the DFN model are stochastically parameterized from geological fracture data and borehole well-test data — a procedure associated with a large number of estimated parameters and hence large uncertainties (Paper I). Therefore, an alternative, simpler and more robust SC-based upscaling method is also suggested (Paper I) and its validity is examined based on how well it can reproduce the results of the more elaborate DFN model. Confidence is gained in hydraulic parameterization of models, if meaningful relations are found between the SC and DFN models.

Finally, the hydro-mechanical effects were considered in two ways: (i) first, in terms of improving the parameter estimation of fracture transmissivities in DFN models by accounting for an anisotropic in situ stress regime in an otherwise hydrology-based probabilistic parameterization process (Paper III) and (ii) second, in evaluating of the effects from thermal stresses in the repository near-field on the regional-scale flow and transport (Paper IV). In the latter study, the thermo-mechanical effects were first modelled separately, and the results were then transferred to the hydrological DFN model.

In the following sections these different subtopics are addressed in more detail.
4. Upscaling of hydraulic data (Paper I)

4.1 Methodology

The first objective was to investigate the possibility to approximate the hydrometry of the fracture networks by means of continuum conductivities at some suitable block scale, which then can be used as the support scale of the regional-scale stochastic continuum models. The second objective was to compare the principles of the DFN and SC approaches in such upscaling. This comparison was undertaken as weaknesses exist in the hydraulic parameterization of both approaches, and confidence could be gained if meaningful relations can be established between the two methods. More specifically the following questions were addressed in the comparison: (i) can a SC-based upscaling reproduce the flow results of a DFN model, and if so, (ii) how should the SC-model be parameterized in a meaningful way.

4.1.1 DFN-based upscaling

A classical DFN-based upscaling approach (Section 2.5.3) was first used to establish the validity of continuum approximation at some block scale. The FracMan/MAFIC [Dershowitz et al. (1998); Miller et al. (1999)] software were used for this. The BART Baecher model was selected to generate 3-D fracture networks according to geological fracture data and hydraulic borehole interval data (Andersson and Knight, 2000). Fracture transmissivity was estimated in a probabilistic analysis of the hydraulic borehole data (eq. 2), based on the method of Osnes et al. (1988).

Statistical distributions of fracture network data were available for fracture orientations, lengths, density, and connectivity. These have been compiled from 2-D and 1-D geologic observations. Therefore the statistics need to be extrapolated into a 3-D network. A 3-D fracture radius distribution was extrapolated from the given 2-D trace length distribution (Nirex, 1997a) using methods of Pigott (1997) and Barton (1995). The 3-D fracture area per volume intensity, \(P_{32}\), (Dershowitz and Herda, 1992) was calibrated from 2-D fracture density in trace maps and fracture frequency in boreholes (Nirex, 1997b-c). A sample realization is shown in Fig. 1a and further details on its generation are given in Paper I.
Owing to the incompleteness of the data set available, three important assumptions were made: (i) no correlation between aperture and fracture length (c.f. de Dreuzy et al., 2000), (ii) statistically homogeneous fracture density (c.f. Bour and Davy, 1999), and (iii) four borehole interval transmissivities exceeding the detection limit $10^{-9}$ m$^2$/s, were treated as equal to this limit. It should be noted that other assumptions are possible as well. However, as a general principle, it was decided that without inference from the data given, basic assumptions should be favoured over more complex ones (e.g., the principle of Ockham’s razor). It should also be noted that these assumptions favour the possibility of continuum approximation.

4.1.2 SC-based upscaling

Next, the SC framework was used to explore if the upscaling results of the DFN approach can be reproduced in a much simpler way. As discussed earlier, the classical SC method (Neuman, 1987) operates with hydraulic data “as measured” without accounting for fracture details and its support-scale is taken as the sealed borehole interval of the well-test. Two uncertainties exist in this approach, namely: (i) the tests relate to unknown rock volumes and (ii) their continuum approximations remain unverified. Therefore, two major enhancements were considered to improve the performance of the classical SC approach. These were: (i) introducing a conductivity-dependent correlation structure to reflect fracture connectivity of the medium, and (ii) considering that the size of the rock volume tested may vary with the conductivity of each sealed borehole section. The rationale for considering conductivity-dependent support-volumes for the hydraulic data is that these come from transient well-tests conducted during a finite test period (90 min). Thus it may be expected that during this time period, flow propagates further in a highly permeable zone than in a low-permeable zone.

The SC upscaling approach was performed as consistently to the DFN approach as possible (Fig. 1). A cubic domain was used with the same size as for the DFN-based upscaling. The grid was discretized by cubic elements with side-lengths equal to the borehole intervals. Each element was stochastically assigned a conductivity value $K_e$ based on the hydraulic data. The element conductivities were correlated by an exponential variogram $\gamma$,

$$\gamma(h') = 1 - \exp\left(-\frac{3h'}{a(K_e)}\right), \quad (8)$$

where $a(K_e)$ is the correlation range [m] for an element with conductivity $K_e$ [m/s], and $h'$ is the lag distance [m]. The correlation length, $a(K_e)$, was treated as a fitting parameter that may vary with conductivity, $K_e$. This correlation structure was assumed anisotropic, i.e., it may assume different mag-
nitude in its two principal directions. Furthermore, the principal directions in correlation were assumed to coincide with those of conductivity anisotropy, $K_1$ and $K_2$, as determined by the DFN simulations. The two principal correlation structures are therefore referred to as $a_{K_1}(K_e)$ and $a_{K_2}(K_e)$ (Fig. 1).

The sampled rock volume for each hydraulic test was estimated by flow simulations. The volume was assumed cylindrical and be defined by the height of the sealed borehole section and the “radius of influence” of the test. The influence radii, $r(K_e)$, of the tests were estimated by simulating the hydraulic tests numerically using the radial-symmetric flow equation (Freeze and Cherry, 1979)

$$\frac{\partial^2 h}{\partial r^2} + \frac{1}{r} \frac{\partial h}{\partial r} = \frac{S}{T} \frac{\partial h}{\partial t}, \quad (9)$$

where $S$ is storativity [-], $T$ is interval transmissivity [m$^2$/s], and $h$ is hydraulic head [m]. Storativity data were not available, and therefore it was assumed constant for all well-tests. The radius of influence, $r(K_e)$, was defined as the radial distance where, at the end of the simulated experiment, the increase in hydraulic head is 1% of the initial injection pulse.

A simple way was used to account for the different support volumes of the different well-tests. In the standard SC approach, all hydraulic data are weighted equally when determining the input conductivity probability distributions. In the present approach the hydraulic data were weighted by their “test volumes”, such that a conductivity value sampling a larger rock volume was given a proportionally larger frequency of occurrence in the input distribution.

Figure 1. Upscaling hydraulic conductivity by flow simulations for various orientations, using a) the classical DFN-based approach and b) an enhanced SC-based approach (modified from Paper I).
Directional conductivities $K(\theta)$ were determined by flow simulations (for boundary conditions equal to the DFN approach) for various orientations $\theta$ between the gradient and the principal direction of correlation, $\zeta$ [Fig. 1; eqs. (4 and 5)]. The correlation ranges, $a_{K_1}(K_e)$ and $a_{K_2}(K_e)$, were fitted by matching the directional conductivity distributions from 1000 simulated SC realizations to the previously simulated 150 DFN realizations. The matching addressed the agreement between (i) the geometric mean and standard deviation of the major and minor conductivities, $K_1$ and $K_2$, and (ii) the overall continuum versus non-continuum behaviour. This was studied for three different conductivity input distributions: 1) the “original case” with data directly as measured, 2) “simulated rescaling”, as weighted by simulated support volumes, and 3) “intermediate rescaling.” The last scenario was intended for the case that neither of the two previous scenarios can reproduce the DFN upscaling results.

4.1.3 Hydraulic correlation structure beyond block scale

The previous analysis addressed the connectivity and correlation structure within block-scale rock volumes. In order to transfer the upscaled conductivity data to a regional SC model, the correlation of hydraulic properties that possibly extends beyond the continuum block scale ($\Delta x_{DFN}$) must also be addressed. The method used to estimate this larger correlation structure is not considered a key finding in this thesis. It was mainly used for practical reasons, as the only spatial correlation information available was the configuration of borehole data at the 1.56 m scale. However, as the approach is not explained in any of the appended Papers I-IV, it is for readability briefly summarized here, to explain how the correlation structure of the regional-scale SC conductivity fields was determined (Section 6).

In this approach the experimental variogram of the available borehole data was also upsampled to be compatible with the continuum block-scale conductivities, through the following simulation procedure:

1. An experimental variogram was determined from the original well-test data (1.56 m scale)
2. Multiple SC realizations were generated at a support scale equal to the scale of the test intervals (1.56 m), based on the well-test data and the previously determined variogram. These conductivity fields were larger than the continuum block scale $\Delta x_{DFN}$.
3. A coarser grid was superimposed over the correlated conductivity fields (1.56 m scale), to group the data into blocks (7.8 m scale).
4. Flow was simulated across each of these well-test data groups to determine their equivalent block conductivity at the 7.8 m scale.
5. Each group of well-test data in the original fine-scaled conductivity fields (1.56 m) was replaced by their equivalent 7.8 m block-scale conductivity, to form a coarse block-scale conductivity field.
6. A new upscaled variogram was determined from the coarse conductivity field (with block-size elements).

4.2 Results

4.2.1 DFN-based upscaling

The DFN-based upscaling results were evaluated in terms of effective conductivity as a function of rotational angle, eq. (4), for 150 fracture network realizations. The conductivity tensor of an ideal continuum medium, eq. (5), was fitted to the directional conductivities of each realization (e.g., Fig. 2). Based on these fits, the realizations were divided into three categories: non-continuum, acceptably continuum, and continuum type. At a block scale of 7.5 m, only 5% of the fracture networks were classified as non-continuum. Therefore, the continuum approximation at this block scale was judged reasonable.

Also at this 7.5 m-block scale, the obtained EPM conductivity displays stochastic variability, in terms of $K_1$, $K_2$, and $\xi$, between the different DFN realizations. Therefore, the EPM block scale should not be confused with a representative elementary volume (REV; Bear, 1993). Furthermore, for later application in a regional-scale model its properties must consequently be transferred in an SC framework, rather than by a deterministic continuum approach. The EPM conductivity appears isotropic, i.e., no preferential orientation could be observed in the obtained $\xi$.

Figure 2. Simulated directional conductivities, $K(\theta)$, for a typical continuum-type DFN realization and its fitted continuum tensor, $K_{EPM}(\theta)$ (from Paper I).
4.2.2 SC-based upscaling

The simulated radius of influence of the well-tests, \( r(K_e) \), was found to clearly increase with \( K_e \) (Fig. 3a). However, \( r(K_e) \) cannot be established for \( K_e > 10^{-11} \text{ m/s} \), as the pulse has dissipated to such an extent that it does not exceed 1% at any radius, not even inside the borehole. This result is in excellent agreement with the reported borehole pulse-recovery data (Armitage et al., 1996; Paper I). It was therefore assumed that the injected water volume was insufficient for sampling larger rock volumes than that obtained for \( K_e = 10^{-11} \text{ m/s} \); hence a constant radius was assigned for \( K_e > 10^{-11} \text{ m/s} \) (Fig. 3a).

In the subsequent upscaling flow simulations, neither the “original hydraulic data”, nor the “weighted data” were able to reproduce the results of the DFN-based upscaling (Section 4.2.1). Instead, a less pronounced “intermediate rescaling” (dashed lines; Fig. 3) was best suited.

![Figure 3](image)

**Figure 3.** Simulated rock volumes relating to hydraulic tests a) normalised influence radius depending on borehole interval conductivity on log-log-scale, and b) resulting density function of hydraulic data, weighted by “sampled rock volume” (modified from Paper I).

A main finding in this approach was that the fitted correlation structures of the SC model, \( a_{K_1} \) and \( a_{K_2} \), resemble the density function of fracture transmissivity of the DFN model (c.f. Figs. 4a and 4c).

![Figure 4](image)

**Figure 4.** Results of the oriented correlated SC approach a) fitted principal correlation structures as function of element conductivity, b) comparison of resulting EPM conductivities (\( K_1 \) rotated to the horizontal), and c) fracture transmissivity density distribution (modified from Paper I).
It was also noted that the continuum approximation of conductivity was somewhat worse in the SC approach. The reason is that the mesh of the SC model is too coarse, and therefore its resulting $K(\theta)$ more easily deviates from a tensorial transformation (c.f. SC and DFN results; Fig. 4b).

4.2.3 Upscaled variogram for block scale conductivity

Fig. 5 shows the underlying 1.56 m scale borehole well-test data used in this study. It also shows the data transformed into indicator values, where 1 refers to so-called flowing features and 0 refers to background permeability. This indicator analysis (e.g., Deutsch and Journel, 1998) was used as the data set has a bimodal appearance (Fig. 6a), where the measurements related to flowing features form one group and the background permeability forms another. The standard experimental variogram and the indicator variogram have a similar appearance (Fig. 6b). This implies that the standard variogram is dominated by the correlation between these two sub-populations and may be unsuitable for the current data. Therefore, indicator correlation was used to generate the input conductivity fields for the variogram upscaling studies.

![Figure 5. Hydraulic borehole data (colour scale) and its transformed indicator values (black/white scale).](image)

![Figure 6. Hydraulic well-test data a) histogram of estimated interval conductivity and b) its experimental variogram compared to an experimental indicator variogram.](image)

An example of a correlated SC conductivity field based on hydraulic borehole data and its variogram is shown in Fig. 7a along with the corresponding
upscaled conductivity field in Fig. 7b. The final upscaled variogram, estimated from multiple block-scale conductivity fields, is shown in Fig. 8.

Figure 7. Stochastic conductivity fields a) based on the original borehole data (at 1.56 m scale) and correlated by an indicator variogram, and b) upscaled block conductivities (at 7.8 m scale) solved by flow simulations.

Figure 8. Upscaled variogram for block-scale conductivity.
5. Upscaling of solute transport (Paper II)

Two approaches were explored for upscaling of solute transport to the same block scale as found suitable for continuum representation of flow ($\Delta x^{DPN}$). These are: (i) the possibility to define continuum dispersivity tensors at the block scale of interest, and (ii) quantification of non-parametric transit-time ensembles. The latter approach is intended for fractured media where continuum approximation of transport is not possible at the block scale, and a direct method to apply its results in a regional-scale transport model will be described later (Section 6).

It should be emphasised that the aim here was to demonstrate and develop upscaling approaches. Therefore important transport mechanisms such as sorption, matrix diffusion, and within-fracture-plane channelling were not considered. This was done partly due to the lack of such data, and partly to keep the emphasis on the upscaling approaches. However, in a real case, an extension to implement these mechanisms would be relatively straightforward. The transport was therefore studied by tracking passive particles in fracture networks with equivalent hydraulic (uniform) apertures.

5.1 Methodology

5.1.1 Dispersion tensor at block scale

Regional-scale transport modelling is conceptually straightforward in the case where both conductivity and transport are of continuum-type at the same support scale. Therefore, the possibility of finding EPM dispersivities at the scale found suitable for a continuum approximation of flow was studied first. This was done by analyzing particle breakthrough as a function of rotational angle. The criteria set for continuum approximation of transport to be valid were: (i) particle breakthrough must follow an analytical solution of the advective-dispersive equation (ADE), and (ii) its derived EPM dispersivity must, as a function of rotational angle, follow a tensorial transformation.

The particle tracking analysis was modelled in various orientations in a similar way to the upscaling of hydraulic conductivity (Section 4). For each realization, the flow field was first solved in various directions, $\theta$, by gradually rotating the imposed hydraulic gradient in a vertical plane (Fig. 9). The
transport region was embedded in a somewhat larger flow field ("guard zones"; Jackson et al., 2000) to reduce the effects of boundary conditions on transversal particle spreading. Numerous particles were released at the centre of the inflow boundary and collected at outflow boundaries (Fig. 9). Particle transit-time statistics were sampled at various longitudinal distances, times, and orientations, $\theta$, and analyzed to examine if the transport is of continuum-type at the selected block scale.

![Figure 9. Flow and transport regions vertically rotated by an angle $\theta$ to obtain particle dispersion characteristics along with an example of simulated particle trajectories for one realization (from Paper II).](image)

5.1.2 Transit time distributions at block scale

In fractured media where transport often exhibits non-continuum type behaviour, particle tracking and random walk methods are useful upscaling tools. In the approach of Paper II, particle motion is learnt from a block-scale DFN model and its characteristics are then transferred in the form of non-parametric probability distributions to a regional-scale model.

On the regional scale, transverse dispersivity is often considered less important than the longitudinal dispersivity. If transverse dispersivity is neglected, the block-scale transport can simply be quantified in terms of distributions of transit time $t^{DFN}$, eq. (6). These distributions were defined as the time taken for simulated particles to traverse a block scale DFN. The transport in each DFN realization $i$ at the block scale, is characterized by a transit time distribution $g_i(t)$ determined based on a large number (10,000) of particles released for each network realization.
The following measures were taken to ensure consistency of the results in the later application as input for the regional-scale SC model (Section 6):

1. the same DFN realizations, \( i \), were used as for the upscaling of conductivity (Section 4.1.1).
2. the boundary conditions used were identical to those for the upscaling of conductivity (Section 4.1.1).
3. particles were released and collected over the entire inflow, respectively, outflow areas.
4. the distributions were determined in vertical and horizontal directions.
5. the transit times \( t_{DFN}^{ij} \) were determined separately for an upstream region A and downstream region B of the DFN (Fig. 2 in Paper II).

The reason for the last condition was to ensure geometrical consistency between the regional-scale SC model and the DFN models. In the regional-scale model particles must move from one nodal point to another and these nodal points are located in the centre of the numerical elements. Therefore transit times had to be determined separately for the “upstream section” (i.e., from the boundary with higher hydraulic head to the centre of the block) and for the “downstream section” (i.e., from the centre of the block to the boundary with lower hydraulic head) and are denoted as \( A_{ij} \) and \( B_{ij} \), respectively.

To account for a potential depth trend in fracture transmissivity caused by the closing of fractures with increasing stress, block-scale transit-time distributions were determined for the stress-levels at different depths, \( j \). The relationship between stress-induced fracture closure and depth is explained further in Section 7.1.

5.2 Results

5.2.1 Dispersion tensor at block scale

Particle tracking results show, similarly to earlier studies (e.g., Endo et al., 1984), that the simulated breakthroughs appear more heterogeneous than the results of the flow simulations. As an example, the simulated transit time percentiles, \( t_{16}, t_{50} \) and \( t_{84} \), and the corresponding simulated hydraulic conductivity \( K(\theta) \), as a function of the rotational angle, is shown in Fig. 10 for a typical DFN realization. In fact, neither of the DFN realizations studied could be classified as exhibiting continuum-type transport, based on the two criteria set in Section 5.1.1.
Figure 10. Comparison between flow and transport at block scale for a typical DFN realization: a) simulated directional conductivity and b) particle breakthrough percentiles from 10,000 particles, plotted as functions of rotation angle (from Paper II).

5.2.2 Transit time distributions at block scale

The results from the particle tracking simulations were distributions of particle transit times from 100 DFN realizations. These results were organized in a consistent way to enable a correct linkage between block-scale transport and conductivity properties in the later regional-scale simulations. For each DFN realization, \( i \), the vertical and horizontal components of conductivity, \( K_v \) and \( K_h \), are linked to their corresponding four transit time distributions, \( g_{ij}^{(v)}(\tau) \), \( g_{ij}^{(h)}(\tau) \), \( g_{ih}^{(v)}(\tau) \), and \( g_{ih}^{(h)}(\tau) \) by their mutual index \( i \). Furthermore, the calculated transit times within each distribution are ranked in ascending order, from shortest transit time to longest, and given a rank \( m \) that varies from 1 to the total number of particles released. The reason for saving this information is to carry pathway information between elements in the regional-scale particle-tracking model, as will be discussed in more detail later (Section 6). Examples of particle breakthroughs are shown in Paper II.
6. Regional-scale transport (Paper II)

A regional-scale transport model was introduced for fractured media where hydraulic flow, but not transport, can be approximated by EPM properties at some block scale. Its concept is to solve regional-scale flow in a SC framework and to use a random walk procedure for transport calculations. The size of grid elements in the regional model was made equal to the block scale for valid continuum approximation of flow (Section 4). This ensures a consistent transfer of upscaled flow and transport heterogeneity from fracture networks to the regional model, i.e., each grid element was assigned a conductivity value and its corresponding transit time distribution, which were internally linked via their underlying fracture network.

To model transport that may be of non-continuum type at block scale, the possibility of channelling between grid elements must be addressed. Therefore, alternative algorithms for sampling the transit time distributions were introduced and compared. The most reasonable alternative is to incorporate a “transport persistence length” in the algorithm for the sampling of particle transit times.

In the following, the principle for solving the regional-scale flow fields is first described (Section 6.1.1), followed by the solution for solute transport (Section 6.1.3), and the approach used to model channelized transport (Section 6.1.3).

6.1 Methodology

6.1.1 Regional SC flow model

Regional-scale flow fields were solved in a SC framework based on the upscaled block-scale conductivity distributions (Section 4). To ensure a consistent transfer of heterogeneity characteristics in the subsequent particle tracking, the region downstream of the fault zone (Fig. 11) was discretized by elements of equal size to the block scale for valid continuum approximation of flow, $\Delta x^{SC} = \Delta x^{DFN}$ (Section 4). Larger elements were used in the region upstream of the fault zone (Fig. 11), as no particle tracking will take place in this region.
To account for effects of a stress-induced depth trend, the downstream region was also divided into four depth layers. For each layer \( j \), correlated conductivity fields were generated based on block-scale conductivities \( K_{ij} \), up-scaled from a DFN realization \( i \) (Paper I), being subject to the stress regime at the depth level \( j \) (Paper III). The fields were correlated by the up-scaled variogram (Section 4). The mean conductivity was then adjusted to smoothly follow an interpolation of its depth trend, \( K(z) \) (Fig. 11).

Each generated conductivity value \( K_{ij} \) was indexed to its actual network realization of origin \( i \), and stress-level \( j \), in order to link each element to its corresponding particle transit time distribution \( g_{ij}(r) \). The steady-state flow fields were solved for 30 such regional-scale conductivity realizations. An integral finite difference-based code, TOUGH2 (Preuss et al., 1999), was used to solve the flow fields.

### 6.1.2 Particle random walk

Regional-scale transport was modeled in terms of a random walk through the SC flow fields. The random walk was discretized in terms of block-scale steps across the elements of the SC flow fields. These particle steps were directed by the advective fluxes between adjacent elements. The probability for choosing a particular route is weighted by the relative magnitudes of the fluxes in corresponding directions. The time taken for a particle step to traverse an element with conductivity \( K_{ij} \) was sampled from its particular block-scale transit time distribution \( g_{ij}(r) \), which were linked via their underlying DFN (Section 5).

The sampled transit times were re-scaling according to its local ambient hydraulic gradient. This scaling was based on the well-known relationship between velocity and transit time and expressions for linear flow velocity,
where $\Delta H$ is the drop in hydraulic head over a particle step $\Delta x$, and the superscripts DFN and SC refer to parameters of the fracture networks and those in the regional-scale stochastic continuum model, respectively. The block scales ($\Delta x_{DFN}$ and $\Delta x_{SC}$) are by definition the same. At the middle of each layer $j$, the conductivities ($K_{DFN}$ and $K_{SC}$) and effective flow porosities ($\phi_{DFN}$ and $\phi_{SC}$) are also equal by definition. However, special care was taken at intermediate depths, $z$, where the mean conductivity in the SC model follows the interpolated depth trend, $K(z)$.

Based on the cubic law, eq. (1), effective porosity was assumed proportional to fracture aperture, and its block conductivity to follow the aperture with a power of 3. Therefore, according to eq. (10), a transit time at an intermediate depth, $z$, was adjusted by the conductivity-depth trend with an exponent of $2/3$. Furthermore, to attain full consistency in the configuration of boundary conditions for the SC and DFN models, a particle step was split into two sequences: the “downstream section” B of the present element and the “upstream section” A of the subsequent element (Paper II). Equation (10) then becomes

$$
\tau_{SC} = \frac{K_{DFN}/\phi_{DFN}}{K_{SC}/\phi_{SC}} \frac{\Delta H_{DFN}/\Delta x_{DFN}}{\Delta H_{SC}/\Delta x_{SC}} \tau_{DFN},
$$

(10)

where $\Delta H$ is the drop in hydraulic head over a particle step $\Delta x$, and the superscripts DFN and SC refer to parameters of the fracture networks and those in the regional-scale stochastic continuum model, respectively. The block scales ($\Delta x_{DFN}$ and $\Delta x_{SC}$) are by definition the same. At the middle of each layer $j$, the conductivities ($K_{DFN}$ and $K_{SC}$) and effective flow porosities ($\phi_{DFN}$ and $\phi_{SC}$) are also equal by definition. However, special care was taken at intermediate depths, $z$, where the mean conductivity in the SC model follows the interpolated depth trend, $K(z)$.

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\[
\tau^{SC}(z) = \left( \frac{E[K_j]}{K(z)} \right)^{2/3} \left( \frac{\tau_{DFN}^{b, DFN}}{\Delta^2 H^{SC}} + \frac{\tau_{DFN}^{A, DFN}}{\Delta^2 H^{SC}} \right) \Delta H_{DFN},
\]

(11)

where $\tau_{DFN}^{b, DFN}$ is a block-scale transit time of DFN realization $i$ in layer $j$, $i'$ refers to the underlying DFN realization of the subsequent downstream element, the indices A and B refer to upstream, respectively, downstream sections, $E[K_j]$ is the mean upscaled block conductivity in the same layer, and $K(z)$ is the interpolated mean conductivity at other depths $z$.

6.1.3 Consideration of channelling

For media where block-scale transport is of non-continuum type, it is unreasonable to sample the transit times of neighbouring blocks independently. The reason is that independent sampling of sequential particle steps implicitly assumes that flow paths mix completely at the interfaces between neighbouring elements. Media that exhibit non-continuum-type transport at some block scale implies a lack of mixing of the flow-channels. Therefore, a possible continuation of transport paths beyond block scale should be considered in cases of incompletely mixed transport. In other words, particles that travel along fast paths in one element may continue to travel along fast
paths in the next, and vice versa for slow particles [cf. Parney and Smith (1995); Benke and Painter (2003); Tsang and Neretnieks (1998)]. This means that, to some extent, the sampling algorithm should consider previously sampled particle steps.

To some extent, the model already considers spatially correlated transport owing to the correlated conductivity field. However, this arises from variable bulk-flow in the regional-scale field and does not take into account the fracture-geometry-induced channelling of transport pathways, which may persist over several elements. Therefore two alternatives were examined to consider such “additionally channelized transport.”

One alternative was to introduce a “dispersion level” $|\Delta n_{\text{max}}|$ that is intended to reflect limited mixing of flow paths at element interfaces. In this alternative, the “dispersion level” controls the allowed velocity change when a particle crosses an element interface. This dispersion level was sampled from a triangular probability distribution with a zero mean, thus giving a particle a higher probability to continue in the next element with a velocity of similar magnitude as before.

The second alternative was to introduce a “transport persistence length”. Here, a particle maintains its velocity over a distance of $N$ successive elements, after which paths were assumed to mix, and new particle velocities and persistence lengths were sampled independently. Channelized transport was examined for various average “transport persistence length,” $N_d$.

These two alternative concepts were used to describe varying degrees of channelized transport. To quantify the effect of channelized transport in terms of macro-scale dispersion, regional-scale particle breakthroughs were fitted to analytical solutions of the ADE. The solution for one-dimensional breakthrough after an instantaneous pulse injection (e.g., Käss, 1998) can be expressed for $n_p$ released particles as

$$n(L,t) = \frac{n_p}{t_0} \exp \left[ \frac{1 - \frac{t}{t_0}}{4 \frac{t}{Pe \ t_0}} \right]$$

where $n(L,t)$ is the number of particles at distance between injection and observation $L$ and at time $t$, $n_p$ is the total number of particles released at the source, $t_0$ is the mean transit time, and $Pe$ is the Peclet number ($Pe = \frac{vL}{D_L}$, where $D_L$ is the longitudinal dispersion coefficient, and $v$ is the mean flow velocity).

Different levels of channelized transport were modelled using the ‘dispers- sion level’ mixing and ‘transport persistence length’ concepts, releasing $10^6$ particles each time. This was examined in 30 SC flow realizations.
6.2 Results

6.2.1 Regional-scale flow fields for particle random walk

The random-walk approach was applied for the given field data to analyze its regional-scale particle breakthrough behaviour for the different channeling alternatives. An example result of the particle random walk is shown in Fig. 12. The particle breakthroughs of the various cases were fitted to analytical solutions of the 1-D ADE, to analyze the effect of transport channeling on the effective macroscale dispersion coefficient.

![Simulated regional-scale particle breakthroughs for the minimum level of channelized transport.](image)

6.2.2 Channelized transport and macro-scale dispersion

The obtained particle breakthroughs for the different channelling alternatives were compared (Fig. 13). Both alternatives, ‘dispersion level’ mixing at element interfaces (Fig. 13a), and ‘transport persistence lengths’ (Fig. 13b), appear able to describe varying degrees of channelized transport. The results show one of the interesting findings of Paper II, namely that regional-scale particle breakthroughs seem to be of continuum-type, in spite of exhibiting non-continuum appearance at block scale. This allows analytical solutions of the 1-D ADE to be reasonable fitted to the particle breakthroughs; in particular for the concept of ‘transport persistence,’ its different levels of channelized transport $N_e$ (Fig. 13b), seem well-related to various Peclet numbers when fitted to the ADE (Fig. 13c).
Figure 13. Simulated particle breakthroughs: a) for various ‘dispersion levels,’ $|\Delta m_{max}|$, and b) for various average ‘transport persistence,’ $N_A$, compared to c) analytical solutions of the 1-D ADE for various Pe numbers, eq. (12) (from Paper II).

Additionally, a linear dependency was found between the imposed average “transport persistence length” (quantified by a number of elements $N_A$), and the EPM macroscale dispersion coefficient, $D_L$ (Fig. 14). This was expressed as

$$D_L = D_0 + N_A D_{LB},$$  \hspace{1cm} (13)

where $D_0$ is the background dispersion and $D_{LB}$ is a representative block-scale dispersion coefficient. The physical interpretations these two parameters, and their derivation from block-scale data will be discussed later (Section 8.2).

Figure 14. Average longitudinal macroscale dispersion coefficient, $D_L$, as a function of average ‘transport persistence,’ $N_A$ (from Paper II).
7. Accounting for THM effects (Papers III and IV)

Coupled THM processes imply complex, continuing, mutual interaction between the different processes (Tsang, 1987). A coupled system implies that one isolated process can not be independently predicted with full confidence (Jing et al., 1995). However, in this study the aim was to provide simple estimates of the relative importance of THM effects on flow and transport. Therefore, the THM coupling was studied from a hydrological viewpoint in its simplest form by looking sequentially at the T→M→H processes. In other words, a final thermal state was modelled separately to determine a final mechanical state, which in turn defines the hydraulic state.

Two aspects were examined: (i) use of stress data to obtain a better estimate of fracture transmissivities than can be obtained from well-test analyses alone (Section 7.1.1), and (ii) a sensitivity study to estimate the relative importance of considering THM effects from thermal heating on regional-scale transport (Section 7.1.2).

7.1 Methodology

7.1.1 Combining rock-mechanical and well-test data in the hydraulic parameterization of fractures (Paper III)

The hydraulic parameterization of DFN models is often based on either hydraulic data, or rock-mechanical data, but rarely on both. The probabilistic analysis of well-test data is a sophisticated method to provide an estimate of the variability in fracture transmissivity (Section 2.4.1). However, it does not infer any physically-based explanation for the estimated variability. If the variability to some extent relates to site-specific hydro-mechanical conditions, it should be considered in the hydraulic parameterization. Therefore, a new method was developed to combine hydrological and rock-mechanical data in the hydraulic parameterization of DFN models.

First, the transmissivity distribution for fractures intersecting a borehole is estimated using the standard probabilistic analysis of well-test data, eq. (2). Next, the effect of in situ stress is incorporated by considering fracture
transmissivity, $T_f$, to consist of two independent components: one deterministic stress-dependent mean component $\bar{T}$, and one stochastic variability component, $t' \log T_f \equiv \log \bar{T}(\sigma_e) + \log t' . \tag{14}$

An empirical fracture-closure relationship was derived for the mean transmissivity component, $\bar{T}$,

$$\bar{T}(\sigma_e) \approx \frac{T_0}{(1 + \alpha_e)^\gamma}, \tag{15}$$

where $T_0$ is the mean transmissivity at zero effective stress, and $\sigma_e$ [MPa] is effective normal stress. This relationship was based on laboratory loading-unloading tests of core data (NGI, 1993). The fracture transmissivities of multiple networks (in total $2.5 \times 10^6$ fractures) were then calibrated to satisfy eqs. (2, 14, and 15). This requires that: (i) each fracture transmissivity depends on its orientation versus the stress regime, eqs. (14 and 15), and (ii) the fracture transmissivity statistics as sampled by a vertical borehole must equal its estimated distribution in eq. (2). In other words, the criterion set for a successful calibration was that both the hydraulic and the hydro-mechanical data are honoured (further details are given in Paper III).

The borehole orientation versus the stress regime must also be considered in this procedure. For example, a vertical borehole has a sampling bias towards horizontal fractures and as a result its sampled fracture population may mainly reflect the vertical stress. A parsimonious numerical method was suggested to distinguish the fracture population sampled by the borehole from its total population. The probability of a fracture $f$ to be intersected by a vertical borehole was approximated by

$$P_f \approx \frac{A_L + L_L \times r_w}{A}, \tag{16}$$

where $A_L$ is the horizontally projected area of the fracture, $L_L$ is its horizontally projected circumference, $r_w$ is the borehole radius, and $A$ is the total horizontal area of the DFN block available for borehole sampling. The expected transmissivity distribution detected by a randomly-located vertical borehole was then approximated by weighting all fracture transmissivities within the sampled DFN block by their intersection probabilities, $P_f$.

To evaluate the effect of stress-dependent fracture hydraulics in terms of block-scale conductivity, the DFN-based upscaling (Section 4.1.1) was carried out for multiple realizations subject to stress-regimes at different depths.
7.1.2 Effect of thermal stress in a repository near-field (Paper IV)

A repository is a considerable perturbation of the current geohydraulic system and alters the ambient conditions from their original in situ state (Tsang et al., 2000). Two changes are of mechanical (M) character, namely those due to tunnel excavation and swelling of the backfilling material. In addition there are thermo-mechanical (TM) effects, due to heat emission of the waste. Their significance on predicted radionuclide transit times was examined, in relation to the heterogeneity-induced uncertainty of the initial state, for a hypothetical repository. This was investigated in terms of a sensitivity study using what is called sequential uncoupled modelling according to the notation of Tsang (1987).

The two TM processes were modelled with the 2-D UDEC software (Itasca, 2000) using simplified assumptions and parameterization (Paper IV). The TM-effects on the stress field were determined for two separate cases: (i) tunnel excavation followed by a backfilling swelling pressure of 2 MPa, and (ii) 100 years of heat emission. The following procedure was then used to transfer the TM-model results to a hydraulic model and to estimate their impact on regional-scale transport:

1. The TM-change in the stress-field was expressed in terms of normal stress acting over fractures at various locations and orientations.
2. The changes in the normal stresses acting on fractures were related to changes in fracture transmissivity using the fracture-closure relation, eq. (15). The effect on transmissivity depends on the orientation of a fracture and its distance from the repository.
3. The impact on block-scale conductivity was quantified by hydraulic upscaling for a number of DFN realizations where fracture transmissivity was adjusted from their original values.
4. Regional-scale transport was modelled by a simplified particle tracking approach. The particle tracking was performed for SC flow fields based on both the original block-scale conductivity and the TM-altered conductivity distributions.
5. Finally, the TM effect on regional-scale transport was estimated by comparing particle breakthroughs from the original SC flow fields to those obtained for TM-modified SC flow fields.

The reason for using a “simplified particle tracking approach”, was that here, the analysis of TM effects was prioritized over the effects of channelling and heterogeneity. In this “simplified version” a single transit time distribution was used. This distribution was assembled from the transit times of multiple DFN realizations (Section 5) and assumed to represent the transport characteristics of the “average” fractured rock. The transit time for a step in the
random walk through the regional SC-flow field was sampled from the joined distribution and rescaled according to

\[ \tau_{\text{SC}} = \left( \frac{K_{i}^{\text{DFN}}}{K^{\text{SC}}} \right)^{2/3} \frac{\Delta H^{\text{DFN}} / \Delta x^{\text{DFN}}}{\Delta H^{\text{SC}} / \Delta x^{\text{SC}}} \tau_{i}^{\text{DFN}}, \]

where \( \tau_{i}^{\text{DFN}} \) is the transit time through a random DFN realization \( i \) with equivalent conductivity \( K_{i} \), and \( K^{\text{SC}} \) is the harmonic mean of the two adjacent element conductivities involved in one particle step in the SC model. The element conductivities in the SC model vary from element to element due to: (i) variability in block-scale conductivity, (ii) depth trend in stress resulting from the TM-modelling, and (iii) the repository-induced TM effects. The conductivity depth trend used here relates to TM results, and was therefore different from the depth trend in Section 6, which uses in situ-stress data. Further details are given in (Öhman et al., 2004).

7.2 Results

7.2.1 Including stress regime in hydraulic parameterization

In its application to field data, the introduced calibration method appears practical for estimating fracture transmissivities honouring both hydraulic data and rock-mechanical data. This calibrated fracture transmissivity depends on the depth and orientation of a fracture in a depth-dependent, anisotropic stress-regime.

The impact of the new approach was quantified by comparing the variability of the different components of eq. (14) in terms of their standard deviation of log-transformed fracture transmissivity, \( s_{\log T} \). For the field data analyzed here, the variability of the stress-induced component \( T \) was small (\( s_{\log T} = 0.18 \)) relative to that of the stochastic component \( t' \) (\( s_{\log T} = 1.20 \)). This implies that only part of the variability estimated in the probabilistic analysis can be related to the anisotropic stress regime. Furthermore, the total variability of stress-adjusted fracture transmissivity \( T_f \) (\( s_{\log T_f} = 1.216 \)) is larger than the variability that can be inferred by the probabilistic approach, alone (\( s_{\log T_f} = 1.210 \)). This shows the inability of boreholes in reflecting the full 3-D characteristics of fracture networks.

The net effect of the new approach, relative to the standard probabilistic approach, eq. (2), is also demonstrated in the DFN-based upscaling results (Fig. 15). Its impact is expressed in terms of mean anisotropy in block-scale conductivity, i.e., stress-adjusted block conductivity normalised by the conductivity based on the probabilistic approach alone, eq. (2). The principal
components of conductivity ($K_1$, $K_2$, and $K_3$) are found to be parallel to those of stress ($\sigma_1$, $\sigma_2$, and $\sigma_3$). The vertical anisotropy (Fig. 15a) is larger than the horizontal anisotropy (Fig. 15b).

![Figure 15](image)

*Figure 15. Anisotropy effect on block-scale conductivity due to stress-regime: a) rotation in horizontal plane and b) rotation in a vertical plane (from Paper III).*

### 7.2.2 Thermal stresses in the repository near-field

The TM-model results indicate that the modelled effects of repository excavation and backfilling swelling pressure have little impact on the stress field. The maximum TM effect appears to be at 100 years of heat emission. At this time, thermal stresses have reduced block-scale conductivity by a factor of two in the repository near-field (Fig. 16). This is a very similar finding to that of Min (2003). The TM-effect on block-scale conductivity is found to be isotropic and to have non-significant effects on the validity of continuum approximation. The TM-effect on block-scale conductivity levels out at distances exceeding 180 m from the repository (Fig. 16). Beyond that distance, it was assumed to have dissipated.
Figure 16. Change in fracture transmissivity, a fitted trend and resulting block-scale conductivity for various repository distances (from Paper IV).

In terms of particle tracking results, the TM effects on regional-scale were generally low. At 100 years of heating, the transit times were typically delayed approximately by 5%. More detailed results are given in Paper IV.
8. Discussion

8.1 Hydraulic upscaling

8.1.1 Validity of stochastic continuum approximation
The DFN-based upscaling of flow indicates that continuum approximation of flow was possible at a support scale of 7.5 m for the present data. At this support scale only 5% of the DFN realizations were classified as non-continuum type and therefore this scale was selected for the further regional-scale analyses in a stochastic continuum framework. It should be pointed out that to accurately account also for the 5% non-continuum type fracture networks, somewhat enhanced approaches could be used, such as overlapping-continua models (e.g., Berkowitz, 2002) where fractures would be superimposed to the regional-scale SC model.

It is also important to note that the scale of validity the continuum approximation depends on the parameterization of the underlying DFN model. It is know from earlier studies that the parameterization of a DFN model is generally an ill-posed problem with non-unique solutions [Berkowitz (2002); Neuman (1987)] and can be seen also in the derivation of these properties in the present work (Paper I). Therefore different continuum scales may also be obtained with other interpretations of the data (e.g., Andersson et al., 2003). There is also subjectivity in the actual acceptance of the continuum approximation. The deviations from ‘perfect’ continuum behavior can be evaluated with objective functions, e.g., by root-mean-squares errors. However, in the end a subjective decision must also be made on what level of deviation should be tolerable [Min et al. (2004a); Paper I].

8.1.2 The oriented correlated stochastic continuum approach
The developed enhanced SC upscaling approach, where the data statistics are (i) corrected for the variable influence radii of the well-tests and (ii) where different conductivities are allowed to assume different correlation lengths, appears to reproduce the results of the DFN upscaling in a simple, yet meaningful way.
It was found that when generating the input statistics from the hydraulic data, these data must be weighted by some support-scale volume that reflects the volume of the measured domain. The performed numerical well-test simulations indicate that the sampled rock volume increases with borehole-section transmissivity up to a certain threshold \((K_e = 10^{-11} \text{ m/s})\). However, this analysis was made with simplified assumptions (e.g., EPM approximation at measurement scale and the cylindrical flow regime); its results should therefore merely be interpreted as a physically-based motivation for weighting the hydraulic data depending on their element conductivity rather than an accurate account of the phenomenon.

In the subsequent upscaling simulations, it was actually observed that neither the “original hydraulic data”, nor the “weighted data” (based on the numerical simulations) were able to reproduce the results of the DFN-based upscaling. Instead, a less pronounced “intermediate rescaling” (dashed lines; Fig. 3) was required. At least two factors are likely to have exaggerated the simulated rescaling radius. First, there is a bias as a borehole test can sample a large rock volume of high conductivity, but cannot sample a large volume of low conductivity. Second, the storativity was assumed constant for all borehole data. If storativity increases with conductivity, the differences in radius of influence would be less pronounced.

The main finding in this approach was that the fitted anisotropic correlation structures (correlation length functions for \(a_{K_1}\) and \(a_{K_2}\)) resemble in shape the probability density function of fracture transmissivities of the DFN model (Fig. 4). In other words, the conductivity region where there are most fractures in the fracture network model (Fig. 4c) is the same region that should assigned large correlation lengths in the stochastic continuum model (Fig. 4a). A possible interpretation for this finding is that both the transmissivity distribution and the correlation structures relate to probability of connected flow paths across the block. The DFN has a well-connected “backbone” of short fractures where most have transmissivities in the range \(10^{-13}\) to \(10^{-12}\) m²/s (Fig. 4c). This appears “equivalent” to prescribing block-scale correlation lengths to grid element conductivities in the range \(10^{-13}\) to \(10^{-12}\) m/s. In addition to this back-bone, there are also fractures of higher transmissivity in the DFN. These fractures are less abundant and therefore less likely to form connected flow paths through the DFN. The analogy in the SC framework seems to be assigning conductivity-dependent correlation ranges that are proportional to fracture transmissivity density (or “probability of connected paths”).

8.2 Transport upscaling

As is often found in the case of fractured media, that solute transport appears more heterogeneous than does flow. This was also the case here, for which
reason the non-parametric particle tracking method (Paper II) was introduced, allowing the transfer of the non-continuum block-scale transport to the regional-scale model.

It should be pointed out that, when the block-scale EPM dispersions are replaced by advective particle travel time distributions in the direction of the hydraulic gradient, their transversal dispersivity components are ignored. However, this seems to be of minor importance, given the overall large uncertainties in the estimation of flow and transport properties in fractured media.

8.3 Regional-scale transport

An important consideration in the developed regional-scale particle transport method is the linking of the block transit-time distributions with one another. Different alternatives were tested and the physically most meaningful appeared to be the concept of ‘transport persistence length.’ This alternative can be seen as some kind of additional correlation structure for transport, which is superimposed to its background correlation caused by the correlated conductivity fields. The physical interpretation of this parameter and its potential practical application to field data are further discussed in Paper II.

One of the main findings of the large scale particle tracking analyses were that at the regional-scale, particle breakthroughs seem to be of continuum-type, in spite of exhibiting non-continuum appearance at block scale. Furthermore, a linear dependency was found between the imposed average ‘transport persistence length’ and the macroscale dispersion coefficient $D_L$ (eq. 13). The background dispersion $D_0$ in eq. (13) is always present, even without any imposed channelling (i.e., $N_x = 1$). It can be linked to the dispersivity arising from the underlying correlation of conductivity according to the expression by Gelhar and Axness (1983) [eq. (7) in Paper II]. In the present case $D_0$ has a somewhat larger value than that in the idealized theoretical case. This can be explained by (i) the existence of a depth trend in the regional conductivity, and the facts that (ii) the repository is not a point source and (iii) the transport is not strictly one-dimensional. The representative block-scale dispersion coefficient $D_{LB}$ could be inferred from block-scale particle breakthroughs. It was estimated by the product of the geometric mean of approximate block-scale dispersivities, and the mean velocity from the source to the observation point ($D_{LB} = \alpha_g \times v$).

8.4 THM effects

For the data applied, the stress-induced component was found to have a relatively small contribution to the overall variability in fracture transmissivity
The standard deviations of the two components in eq. (14) were 0.18 and 1.20, for $\log T$ and $\log t'$, respectively. The reason is that the hydraulic data were measured under high stress at large depths (from 635 to 790 m depth), where the nonlinear fracture-closure is less sensitive to stress. An interesting finding is that the calibrated stress-dependent transmissivity has an overall variability, which is somewhat larger than the variability of fractures sampled by a vertical borehole. The reason for this is that the 1-D sampling of a borehole is unable to fully reflect the full characteristics of a 3-D fracture network. Therefore, using the probabilistic approach alone in the interpretation of well-test data, will underestimate the full variability of fracture transmissivity. Also, in the DFN-based upscaling of block-scale conductivity, the principal components of anisotropic conductivity ($K_1$, $K_2$, and $K_3$) were found to coincide with those of stress ($\sigma_1$, $\sigma_2$, and $\sigma_3$), which agrees with field observations [e.g., Carlsson and Olsson (1979); Hermansson (1995); Talbot and Sirat (2001)]. Although these effects are small in the present data, the findings are expected to be of larger importance for low stress-levels, strongly anisotropic stress-fields, borehole-directions parallel to one principal stress, and fracture-network geometries characterized by sets orthogonal to the three principal stresses.

In its present application, only one generalized fracture-closure model was used for all fractures in the present application, regardless of geologic origin, past loading history, depth, or orientation. This is a strong simplification, since fractures are known to display highly deviant responses to stress [e.g., Bandis et al. (1983); Barton et al. (1985); Rutqvist and Stephansson (2003)]. Given a larger rock-mechanical data set, the approach could be easily extended to include set-specific fracture-closure models.

The impact of THM effects on regional-scale transport (Paper IV) is found to be small. As discussed above, the reason for this is that the in situ-stresses are high at the repository depth, and under high stresses the nonlinear fracture-closure relation is less sensitive to changes in stress. Therefore, a moderate change in stress in the repository near-field does not significantly alter the fracture transmissivity. Thus, in the perspective of the long transport times (on the order of 10,000 years in combination with peak temperatures at 100 years), the need for THM coupling in regional-scale transport models is not critical, at least not in relation to the heterogeneity-induced hydraulic uncertainties. This conclusion is in agreement with the general conclusions of the given DECOVALEX task (Andersson et al., 2003).
9. Conclusions

This thesis provides a systematic hybrid framework for the upscaling of flow, transport, and stress-effects in fractured media. All four papers are based on the same data set, and target different aspects relevant in an integrated prediction of regional-scale transport. The data set was not complete and used only as an example. Therefore the main results of the thesis are the integrated approach and the related model developments made, rather than any particular application to the field data.

The approach taken is a so-called hybrid approach where a discrete fracture network (DFN) model is used to estimate equivalent properties of flow, transport and stress-effects at some block scale, which are then transferred in terms of block-scale properties to a regional-scale stochastic continuum (SC) model. The approach relies on a successful continuum approximation of flow, but not necessarily of transport, at some block scale. In the case of the present data the suitable support scale for was found to be 7.5 m.

The following model developments have been made and tested, which has also lead to some new observations concerning the behaviour of fractured media.

- An enhanced SC upscaling approach (Paper I), so-called oriented correlated stochastic continuum approach, has been developed that can successfully reproduce the flow upscaling results of the DFN model in a simpler way. In this method, unlike the classical SC approach, (i) the well-test data are weighted by their corresponding conductivity-dependent test volumes when the statistical input distribution is generated and (ii) the correlation structure is conductivity dependent, i.e., different conductivities may assume different correlation lengths. The most interesting finding when comparing the DFN and SC models is that the density function of DFN transmissivities has a shape which is similar to the conductivity-dependent correlation structure of the SC model. In other words, the conductivity region that has the most fractures in the DFN model should be given the longest correlation lengths in the case of the SC model.

- A new regional-scale particle random walk method has been developed (Paper II). The approach transfers flow and transport properties
A new method has been developed that uses both hydraulic well-test data and in situ rock-mechanical data in deriving fracture transmissivities for DFN models (Paper III). It starts from a probabilistic analysis of well-test results in combination with fracture density data and then incorporates the in situ-stress field by describing the transmissivity of each fracture as a sum of a stress-dependent mean and a stochastic component. The benefit of the new approach is a more complete characterization of fracture transmissivity than can be obtained based on either hydraulic or mechanical data alone. Application to the present data indicated that, for the present data, the variability in fracture transmissivities due to the stress field was small in comparison to the random component. Examples of field conditions where the proportions are likely to be different are also discussed.

A sequential approach to study the importance of the overall THM effects on regional-scale transport in a nuclear repository setting, is also introduced (Paper IV). The TM effects are calculated separately and their impact on fracture transmissivities is transferred to the flow and transport model. For the data set studied, these effects were found to be small in comparison to the uncertainties arising from the overall heterogeneity. The reason is that, at the high in situ-stresses encountered at the repository depth, the non-linear relationship between fracture-closure and stress is not very sensitive to changes in stress. Therefore, in the perspective of the large uncertainties arising from hydraulic heterogeneity, the use of full THM coupling in regional-scale transport simulations appears to be of less importance.

In summary, these methods appear to be promising tools for an improved characterization and modelling of flow and transport in fractured media. Further applications to different types of field data are of great interest.
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I dedicate this to you and to our new family member.
11. Summary in Swedish

Uppskalning av flöde och ämnestransport i sprickigt berg samt bergspänningsens inverkan

Datormodellering av vattenflöde och ämnestransport i sprickigt berg har många tillämpningsområden. Ett av dessa är att analysera säkerheten vid djupförvaring av radioaktivt avfall. I ett flertal länder pågår för närvarande platsunderökningar i syfte att finna lämpliga berggrunder för ett framtida djupförvar. En berggrunds lämplighet bedöms bland annat beroende på dess grundvattenflöde, transportegenskaper för lösta ämnen och bergmekaniska egenskaper, vilka kan utvärderas med hjälp av olika datorsimuleringsmetoder.

För sådana utvärderingar krävs datormodeller som på ett adekvat sätt kan beskriva en bergmassas egenskaper. Ett flertal faktorer försvårar modellbeskrivningen av sprickigt berg. En sådan är bergmassans extremt heterogena egenskaper, vilket i kombination med begränsade platsspecifika data framvångar ett stokastiskt angreppssätt. En annan faktor är att vid storskalig analys måste modellbeskrivningen av bergmassans heterogenitet förenklas på grund av begränsad beräkningskapacitet. En tredje faktor är att flöde och ämnestransport påverkas av bergspännning [s.k. kopplade termohydromekaniska (THM) processer]. Spännningen kan förändras från sitt ursprungliga tillstånd p.g.a. kärnavfallets värmeavgivning som orsakar termisk expansion av berget.

De två konceptuella modeller som studerats här är den diskreta spricknätsmodellen och den stokastiska kontinuummodellen. Spricknätsmodellen kan beskriva sprickors geometri och inbördes förbindelse och är därför överlägsen i att analysera processer på mindre skala (meter). Nackdelen är att den ofta är för beräkningsintensiv för tillämpning på större skalar (kilometer). Den stokastiska kontinuummodellen baseras på en förenklad bild av en bergmassa (ekivalenta kontinuemgenskaper), vilket gör metoden beräkningsnål och praktisk för större skalar. Modellens giltighet kräver att processer i sprickigt berg verkligen kan beskrivas med kontinuumegenskaper. Vid storskalig analys kan därför en s.k. hybrid kombination av de två modellerna användas. I den hybrida metoden bestäms ekvivalenta egenskaper med
hjälp av en spricknätsmodell (s.k. ’uppskalning’ från stokastiska sprickdata), för att sedan, på ett konsekvent sätt, överföras till en stokastisk kontinuummodell.

Det övergripande syftet med avhandlingen var att utveckla metoder för att systematiskt skala upp ekvivalenta egenskaper hos spruckna bergmassor, med avseende på vattenflöde och ämnestransport, och att sedan utvärdera bergspänningsens inverkan på storskalig ämnestransport med den hybrida metoden. Detaljerade mål var att:

1. jämföra grunderna för spricknätsmodeller och stokastiska kontinuummodeller vid uppskalning av hydrauliskt flöde, samt att utveckla en ny uppskalningsmetod baserad på den stokastiska kontinuummodellen,
2. utveckla en uppskalningsmetod för ämnestransport i sprickigt berg för simulering på regional skala, samt att undersöka förhållandet mellan kanaliserad transport och makrodispersion,
3. utveckla en metod för att kombinera bergmekaniska och hydrauliska data vid hydraulisk parametrerings av spricknätsmodeller och
4. utveckla ett övergripande tillvägagångssätt för att utvärdera termomekanisk påverkan på hydraulisk konduktivitet och storskalig ämnestransport för ett hypotetiskt djupförvar av kärnbränsle, baserat på en begränsad mängd plattsspecifika data.

Studien baseras på geologiska och hydrauliska data som bygger på delar av resultaten av platsundersökningarna vid Sellafield i Storbritannien, vilka har genomförts av Nirex UK Ltd.

Andra steget i den hybrida metoden var att bestämma bergets ekvivalenta transportegenskaper på den skala som redan fastställts för flöde (7,5 m). Detta gjordes genom att simulera partiklars väg genom bergmassan och bestämma spridningen i deras uppehållstid. Kontinuumegenskaper kunde sedan utvärderas med en analytisk lösning av den klassiska advektions-dispersions-ekvationen. Ämnestransporten uppsvisade inte ekvivalenta kontinuumegenskaper vid denna skala (d.v.s kunde inte beskrivas på ett förenklat sätt). Därför kvantifierades den istället med diskreta statistiska fördelningar i uppehållstid, för samma spricknätverk som använts för uppskalning av flöde.


För att uppskatta sprickors transmissivitet (vattenledningsförmåga) i spricknätsmodeller används ofta antingen hydrauliska borrhålsdata, eller bergmekaniska data, men sällan båda i kombination. Här användes Osnes statistiska analyseteknik för att först uppskatta en fördelning av spricktransmissivitet från hydrauliska borrhålsdata. Transmissiviteten för en spricka kunde sedan definieras som delvis spänningsberoende och delvis stokastisk, genom ett empiriskt förhållande som baseras på hydromekaniska sprickdata. Detta kalibrerades statistiskt för ett stort antal sprickor (2,5 • 10^6) med en spricknätsmodell. Villkoren var: (i) att transmissivitetsfördelningen som uppskattats med Osnesmetoden bevarades (med hänsyn tagen till att den bild av sprickor som påträffas av vertikala borrhål är statistiskt skev), samt (ii) att varje sprickas transmissivitet beror av djup och riktning i det anisotropa spänningsfältet genom det empiriska förhållandet. Resultaten visade att den nya metoden ger en mer fullständig bild av sprickors transmissivitet, samt att Osnesmetoden underskattar den totala variabiliteten, även om denna effekt är liten för de givna data.
Slutligen kunde den termomekaniska inverkan av ett hypotetiskt djupförvar av kärnbränsle utvärderas med avseende på hydraulisk konduktivitet och storskalig ämnestransport. De termiska bergspännningar som uppkommer av kärnavfallets värmeeavgivning kan simuleras med en separat termomekanisk datormodell. En ökande bergspänning pressar samman sprickor, vilket minskar deras vattenledningsförmåga. Detta kan beräknas genom att använda det empiriska hydromekaniska förhållandet (se ovan). På så vis kunde bergspännningens inverkan på bergmassans egenskaper bestämmas och överföras till den hybrida modellen som beskrivits ovan. Resultaten indikerar att de termiska spännningarna når ett maximum efter 100 år, men att deras inverkan på storskalig ämnestransport är liten, speciellt med hänsyn till övriga osäkerheter.

Avhandlingen presenterar ett systematisk angreppssätt för storskalig analys av vattenflöde och ämnestransport i sprickigt berg under bergspännings inverkan, genom kontinuumapproximation av bergmassans egenskaper. De viktigaste slutsatserna var:

- Med spricknätsmodellering kunde ekvivalenta kontinuumegenskaper fastställas vid skalan 7,5 m för bergmassans vattenflöde, men inte för ämnestransport i bergmassan.
- Storskalig ämnestransport kunde simuleras med en nyutvecklad partikelspårningsmetod för sådana fall där flöde, men inte ämnestransport, upparvisar kontinuumegenskaper på mindre skala (såsom i detta fall). Denna metod kan även beakta bergmekaniska förhållanden samt kanaliserad transport.
- Ett linjärt förhållande fastställdes mellan makrodispersion och produkten av en karakteristisk långd för kanaliserad transport och en representativ dispersionskoefficient. Denna representativa dispersionskoefficient visade sig vara lika med det geometriska medelvärdet av alla approximerade dispersionskoefficienter.
- Genom att beakta bergmekaniska data vid statistisk analys av hydrauliska borrhålsdata, fås en mer komplet bild av sprickors dimensionella hydrauliska fördelning, vilket kan yttra sig i en anisotropisk och djupberoende beskrivning.
- För de givna data visade sig det hypotetiska djupförvarets termomekaniska påverkan ha liten inverkan på storskalig transport, speciellt i jämförelse med de osäkerheter som orsakas av den hydrauliska heterogeniteten.
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