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Methodology for hydrological and hydrogeological modelling of the Forsmark site

Magnus Odén, Sven Follin, Kent Werner

Svensk Kärnbränslehantering AB

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Preface

A series of methodology reports supports the programmes for geoscientific investigations and modelling of planned geological repositories for radioactive waste in Forsmark. The methodology reports include ground elevation and regolith stratigraphy, large geological structures (ductile and/or brittle deformation zones), bedrock thermal properties, rock mechanics properties, bedrock transport properties, discrete fracture network realisations, hydrological-hydrogeological and hydrogeochemical processes, properties, and state variables.

Abstract

Surface-based investigations for a deep geological repository for Sweden's spent nuclear fuel were performed between 2002-2008 at Simpevarp, Laxemar and Forsmark. A series of generic, discipline-specific methodology reports offered the theoretical underpinning for the methods and best practices that should be applied to the various aspects of geoscientific characterization and site descriptive modelling. The generic methodology report for hydrogeological investigations and modelling was based on concepts developed during the construction of the Äspö Hard Rock Laboratory (ÄHRL). Hydrological processes and integrated hydrological-hydrogeological modelling were superficially considered.

The structural-hydraulic characteristics of the bedrock near the ÄHRL are influenced by the regional Äspö deformation zone, which crosses the Äspö island. In contrast, the bedrock investigated for a deep geological repository at Forsmark is situated within a sparsely fractured tectonic lens with very different structural-hydraulic characteristics. For this reason, complementary modelling methodologies were developed for the Forsmark site descriptive modelling using discrete fracture network (DFN) concepts. Though adequate for the site descriptive model and the subsequent safety assessment at Forsmark, SKB identified the need to unify and update the complementary methodologies for DFN modelling to meet expected challenges during the construction of the spent fuel repository and to reflect the state of the art in this increasingly complex field of science. The concepts considered by SKB for future DFN modelling – both historic ones and more novel, including structural conditioning and hydromechanical calibration – are described in a separate methodology report.

This methodology report presents a protocol for integrated hydrological-hydrogeological modelling for a deep geological repository for Sweden's spent nuclear fuel inside the tectonic lens in Forsmark. The protocol strives for consistency between the modelling concepts, and tools, used for groundwater modelling in the bedrock and in the regolith, respectively. The hydraulic interaction between the discretely fractured bedrock and the porous regolith is handled through "upscaling", a form of averaging in which DFN model realisations of the bedrock are transformed into "equivalent continuous porous medium" (ECPM) grid model realisations. In effect, the workflow of the protocol is divided into two stages: a DFN stage and a ECPM stage. Notably, the design of the modelling protocol is independent of the concepts of the underpinning DFN model but expects that the generated DFN model realisations are geometrically conditioned and hydraulically (or hydromechanically) calibrated prior to upscaling. Commonly used ECPM upscaling methods are presented in connection with the protocol.

The protocol recommends that structural-hydraulic data identified in SDM-Dite for the so-called local model domain inside the tectonic lens are considered in the DFN stage, particularly: the hydraulic interferences in the uppermost 150 m of the bedrock, the hydraulic resistance for flow transverse the regional Singö deformation zone, and the linear intensity and transmissivity of open fractures. These conditions influence the conceptual modelling, flow model calibrations, and predictive simulations, including: the spatial distribution of groundwater inflow (recharge) and outflow (discharge) areas, prediction of water table drawdowns during the construction of repository accesses, vertical groundwater fluxes between the ground surface and repository depth, and simulations of particle tracking exit locations.

The protocol proposes that multiple DFN (Discrete Fracture Network) realizations be structurally conditioned and hydraulically calibrated during the DFN stage. Structural conditioning and hydraulic calibration should be based on available borehole fracture logs and hydraulic single-hole and cross-hole (interference) tests conducted within the local model domain characterized in the SDM-Site. Subsequently, several approved DFN model realizations should be upscaled to ECPM (Equivalent Continuous Porous Medium) model realizations in the ECPM stage. These ECPM realizations should then be tested against the same cross-hole tests used for the underlying DFN models. If the results from the upscaled ECPM models are unsatisfactory, this may be due to inadequate geometric resolution (i.e., insufficient discretization) of the selected ECPM grid. To assess whether this is the case, it is recommended to repeat the upscaling using an ECPM grid with higher resolution.

SKB has been using two porous medium flow modelling tools (codes) in parallel since the start of the detailed site investigations at Simpevarp, Laxemar, and Forsmark. The reason is that one code is better suited for handling the earthbound part of the hydrologic cycle – that is, groundwater flow in the regolith, interactions with the atmosphere, and groundwater-surface water interactions – whereas the other code is better suited for modelling groundwater flow and solute transport in the bedrock. Though adequate for the site descriptive model and the subsequent safety assessment at Forsmark, SKB has identified the need to unify the modelling tools for porous media flow modelling to streamline anticipated future modelling challenges during construction and open repository operations. However, at the time of writing this methodology report, the design of the protocol is adapted to the fact that two porous media flow modelling tools are still being used in parallel.

Regarding data for future integrated hydrological and hydrogeological modelling and predictive simulations, new boreholes will be drilled from excavated underground openings to characterize the geometric and material properties of the bedrock adjacent to the openings at different depths. These data are key for the concepts considered by SKB for future DFN modelling described in the separate methodology report for DFN modelling. No new boreholes are planned to be drilled from the ground surface, except in the uppermost bedrock near the planned accesses. However, these boreholes are not intended for geoscientific investigations but for curtain grouting to a depth of approximately 60 m. It is noted that grouting will also be used, when needed, in the short boreholes drilled into the bedrock ahead of the tunnel front to control groundwater inflow. The aspects listed above imply that existing data from past investigations in boreholes drilled from the ground surface will remain key also for future hydrological and hydrogeological flow modelling.

Sammanfattning

Undersökningar för ett djupförvar för Sveriges använda kärnbränsle genomfördes från markytan mellan 2002 och 2008 vid Simpevarp, Laxemar och Forsmark. En serie generiska, ämnesspecifika metodrapporter tillhandahöll den teoretiska grunden för de metoder och bästa praxis som skulle tillämpas inom olika aspekter av geovetenskaplig karaktärisering och platsbeskrivande modellering. Den generiska metodikrapporten för hydrogeologiska undersökningar och modellering baserades på koncept som användes under uppbyggnaden av bergslaboratoriet på Äspö (ÄHRL). Hydrologiska processer och integrerad hydrologisk-hydrogeologisk modellering behandlades endast översiktligt.

Den generiska metodiken för hydrogeologiska undersökningar och modellering baserades på erfarenheter från byggandet av berglaboratoriet på Äspö (ÄHRL). Berggrunden på Äspö genomkorsas av en regional skjuvzon, medan den undersökta berggrunden i Forsmark är belägen inom en tektonisk lins vars geologiska och hydrogeologiska egenskaper skiljer sig markant från de som råder på Äspö. Av denna anledning utvecklades kompletterande modelleringsmetodiker baserade på koncept för diskreta spricknätverk. Även om dessa metodiker var tillräckliga för den platsbeskrivande modellen och den efterföljande säkerhetsanalysen i Forsmark, identifierade SKB ett behov av att enhetliggöra och uppdatera de kompletterande metodikerna för modellering av diskreta spricknätverk för att möta förväntade utmaningar under byggandet av slutförvaret för använt kärnbränsle och för att återspegla den senaste utvecklingen inom detta alltmer komplexa vetenskapsområde. De koncept som SKB för närvarande beaktar för framtida DFN-modellering – både historiska och nyare, inklusive strukturell konditionering och hydromekanisk kalibrering – beskrivs i en separat metodikrapport.

Föreliggande metodikrapport presenterar ett protokoll för integrerad hydrologisk-hydrogeologisk modellering för ett djupförvar för Sveriges använda kärnbränsle inom den tektoniska linsen i Forsmark. Protokollet eftersträvar konsistens mellan de modelleringskoncept och verktyg som används för grundvattenmodellering i respektive berggrund och jordlager. Arbetsflödet är indelat i två steg: en DFN-fas och en ECPM-fas. Den hydrauliska interaktionen mellan den diskret sprickiga berggrunden och det porösa jordlagret hanteras genom ”uppskalning”, en form av medelvärdesbildning där diskreta realiseringar av berggrundens spricknätverk (”DFN”) omvandlas till så kallade ”ekvivalent kontinuerlig poröst medium” (”ECPM”) realiseringar. Det är värt att notera att protokollets design är oberoende av vilket/vilka koncept som används för DFN modellering respektive ECPM uppskalning, men rekommenderar att genererade DFN-realiseringar är geometriskt konditionerade och hydrauliskt (eller hydro-mekaniskt) kalibrerade innan uppskalning till ECPM-realiseringar sker. Vanligt förekommande metoder för ECPM uppskalning presenteras i anslutning till protokollet.

Protokollet fokuserar på strukturella och hydrauliska förhållanden för det så kallade lokala modellområdet inom den tektoniska linsen, särskilt: hydrauliska interferenser i de översta 150 m av berggrunden, det hydrauliska motståndet för grundvattenströmning tvärs den regionala Singö deformationszon, samt linjär intensitet och transmissivitet hos öppna sprickor. Dessa förhållanden påverkar den konceptuella modelleringen, flödesmodellkalibrering, samt olika typer av prediktiva simuleringar, inklusive: rumslig fördelningen av grundvattnets inströmnings- och utströmningsområden, prognoser för grundvattenytans avsänkning under uppförandet av tillfarter, grundvattenflöden på olika djup mellan markytan och förvarsdjupet, samt simuleringar av utströmningsområden vid partikelspårning.

Protokollet föreslår att minst tio strukturellt konditionerade och hydrauliskt kalibrerade DFN-realiseringar etableras i DFN-fasen. Den strukturella konditioneringen och hydrauliska kalibreringen ska baseras på tillgängliga enhåls- och interferenstester som genomförts inom det lokala modellområdet i SDM-Site. Därefter uppskalas minst tre av de geometriskt konditionerade och hydrauliskt kalibrerade DFN-realiseringarna till ECPM-realiseringar. Dessa ECPM-realiseringar testas mot samma interferenstester som de underliggande DFN-realiseringarna. Otillfredsställande resultat från ECPM-realiseringarna kan bero på bristande (otillräcklig) geometrisk upplösning (diskretisering) hos den valda ECPM-griden. För att avgöra om detta är orsaken rekommenderas att uppskalningen upprepas med en alternativ ECPM-grid med högre upplösning.

SKB har sedan de detaljerade platsundersökningarna i Simpevarp, Laxemar och Forsmark använt två modelleringsverktyg (koder) parallellt för flödesmodellering i porösa medier. Anledningen är att den ena koden är bättre lämpad för att hantera den jordnära delen av det hydrologiska kretsloppet, det vill säga grundvattenflöde i jordlager, interaktioner med atmosfären samt grundvatten–ytvatten-interaktioner, medan den andra koden är bättre lämpad för att modellera grundvattenflöde och ämnestransport i berggrunden. Även om detta arbetssätt har varit tillräckligt för platsbeskrivningen i SDM-Site och den efterföljande säkerhetsanalysen SR-Site, har SKB identifierat ett behov av att förena modelleringsverktygen för flödesmodellering i porösa medier för att effektivisera den framtida modelleringen under uppförande och drift av förvaret. Vid tidpunkten för denna metodrapports författande är protokollets utformning dock anpassad till att befintliga modelleringsverktyg fortfarande används parallellt.

Vad gäller data för framtida integrerad hydrologisk och hydrogeologisk modellering samt prediktiva simuleringar, kommer nya borrhål att borras från de utgrävda underjordiska utrymmena för att karaktärisera de geometriska och materialmässiga egenskaperna hos berggrunden i anslutning till dessa, på olika djup. Dessa data är centrala för de koncept SKB överväger för framtida DFN-modellering, som beskrivs i den separata metodrapporten för DFN-modellering. Inga nya borrhål planeras att borras från markytan, utöver i den övre berggrunden nära de planerade tillfarterna. Dessa borrhål är dock inte avsedda för geovetenskapliga undersökningar utan för ridåinjektering till ett djup av cirka 60 meter. Det bör även noteras att injektering kommer att användas, när så krävs, i korta borrhål som borras i förväg framför tunnelborren för att kontrollera grundvatteninflöde. Dessa aspekter innebär att befintliga data från tidigare undersökningar i markytedrivna borrhål fortsatt kommer att vara avgörande även för framtida hydrologisk och hydrogeologisk flödesmodellering.

Contents

1 Introduction

1.1 Background

Surface-based investigations for a deep geological repository for Sweden's spent nuclear fuel were performed between 2002-2008 at Simpevarp, Laxemar and Forsmark. A series of generic, discipline-specific methodology reports offered the theoretical underpinning for the methods and best practices that should be applied to the various aspects of geoscientific characterization and site descriptive modelling.

The generic methodology report for hydrogeological investigations and modelling was based on concepts applied during the construction of the Äspö Hard Rock Laboratory (ÄHRL) (Rhén et al. 1997). Notably, hydrological processes and integrated hydrological-hydrogeological modelling were superficially considered.

Äspö, an island in the Baltic Sea north of Oskarshamn roughly 500 km south of Forsmark, has a very thin layer of regolith, no surface waters, and a rock mass affected by ductile strain and the regional Äspö shear zone, which strikes right across the island. In comparison, the area in Forsmark selected for Sweden's spent nuclear fuel repository, SFK (SDM-Site, SKB 2008), has a very different geological setting with a thicker layer of regolith on top of a lithologically homogeneous rock mass affected by lower ductile strain (a tectonic lens) (Table 1-1). That said, the structural-hydraulic properties of the rock mass within the tectonic lens have significantly different properties above and below c. 150 m depth (see Chapter 3). However, the area in Forsmark selected for an extension of the existing repository for Sweden's low- and intermediate-level radioactive waste, SFR (SDM-PSU, SKB 2013), resembles the geological setting to that of the ÄHRL with a regional shear zone nearby, Singö deformation zone (DZ), and an unevenly distributed layer of regolith on top of a rock mass affected by higher ductile strain (Figure 1-1).

Complementary methodology reports were developed during the site investigations for a spent fuel repository in Forsmark (Bosson et al. 2008, Fox et al. 2007, Follin et al. 2007a,b, 2008, Follin 2008). Groundwater flow was modelled using different flow modelling concepts. One team of modellers focused on ecosystem-related matters using continuous porous media (CPM) models and hydrological time series for calibrating the hydraulic properties of modelled regolith layers. A second team of modellers developed discrete fracture network (DFN) models for the Bedrock system, using borehole tests for the hydraulic calibration along with fracture and porewater chemistry data for subsequent simulations of variable-density groundwater flow, particle tracking, and matrix diffusion calculations.

Though adequate for the site descriptive model SDM-Site and the subsequent safety assessment, SR-Site (SKB 2011), SKB identified a need to unify and update the complementary methodologies for geological DFN modelling (Fox et al. 2007) and hydrogeological DFN modelling (Follin 2008) to meet expected challenges anticipated during the construction of SFK and the extension of SFR, to reflect the state-of-the-art in this increasingly complex field of science. Selroos et al. (2022) present an overview of different DFN modelling concepts, methods and best practices.

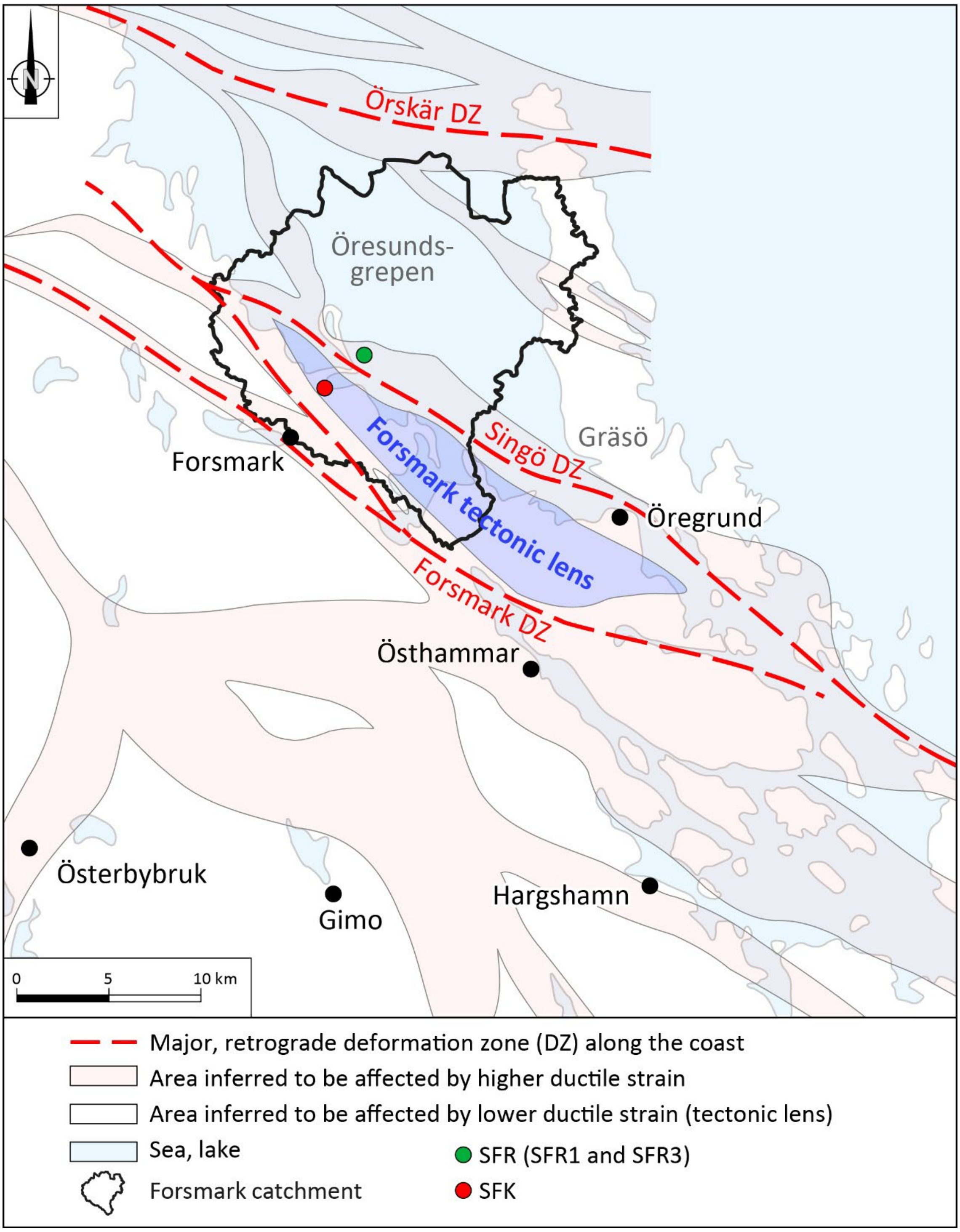

Figure 1-1. *Tectonic lens at Forsmark and areas affected by strong ductile strain along the coastal deformation belt in northern Uppland. The Forsmark tectonic lens is the chosen host rock mass for a deep geological repository for Sweden's spent nuclear fuel, SFK. The bedrock inside this lens is sandwiched between the Singö and Forsmark deformation zones and affected by lower ductile strain. The geological repository for Sweden's low- and intermediate level radioactive waste, SFR, was constructed in the 1980's and is still in operation. SFR is situated close to the Singö deformation zone in a rock mass affected by higher ductile strain. SFR is constructed below the seabed and will be covered by seawater for at least 500 years. Modified after Petersson et al. (2024). In this version the Forsmark catchment is inserted for reference.*

1.2 Methodology reports

A series of methodology reports supports the programmes for geoscientific investigations and modelling of planned geological repositories for radioactive waste in Forsmark. Report numbers (ID), acronyms, and titles are shown in Table 1-1. The acronyms are recommended for internal referencing. This methodology report, HGMM, deals exclusively with site-descriptive modelling, in contrast to some of the other modelling methodologies, e.g., DFNMM and TRPMM.

Table 1-1. Methodology reports for geoscientific investigations and modelling

ID	Acronym	Title
R-20-10	DGMM	Methodology for deterministic geologic modelling of the Forsmark site
R-20-11	DFNMM	Methodology for discrete fracture network modelling of the Forsmark site
R-20-13	RMMM	Methodology for rock mechanics modelling of the Forsmark site
R-20-14	HGMM	Methodology for hydrological and hydrogeological modelling of the Forsmark site
R-20-15	HCMM	Methodology for hydrochemical modelling of the Forsmark site
R-20-16	ERMM	Methodology for elevation and regolith modelling of the Forsmark site
R-20-17	TRPMM	Methodology for site descriptive and safety assessment transport modelling of the Forsmark site
R-20-18	THPMM1	Methodology for modelling of thermal properties of the Forsmark site Part 1 – Recommended data and interpretation methods
R-20-19	THPMM2	Methodology for modelling of thermal properties of the Forsmark site Part 2 – Background and methodology development

1.3 Objectives of this methodology report

This methodology report presents a site-specific protocol for integrated hydrological and hydrogeological modelling of a deep geological repository for Sweden's spent nuclear fuel, located within the tectonic lens at Forsmark (Figure 1-1). The repository will be situated at a depth of approximately 470 metres (around –470 m elevation) within the local model domain shown in Figure 1-2 (SKB 2008). A robust conceptual understanding of the structural and hydraulic observations within this domain is therefore essential to the development of the site-specific protocol. The key observations underpinning the protocol are presented in Chapter 3.

The modelling protocol focuses on the hydraulic interaction between the earthbound flows of the hydrologic cycle inside the local model domain. These flows are labelled the Surface system and the Bedrock system in Figure 1-3. The protocol strives for consistent performance of the flow modelling tools used for the regolith (Surface system) and the bedrock (Bedrock system) regarding simulated groundwater levels (hydraulic heads), spatial distribution of groundwater inflow (recharge) and outflow (discharge) areas, water table drawdowns during the construction of repository accesses, groundwater fluxes between ground surface and repository depth, and exit locations in particle tracking simulations. Approved hydrological-hydrogeological models are essential for other applications, or disciplines, such as radionuclide transport calculations, hydrogeochemistry, and biosphere analyses. Usages of modelling results from the integrated flow modelling are not described in this report, however.

At the conclusion of SDM-Site (SKB 2008), the flow modelling of the Surface system and the Bedrock system were not fully integrated, primarily due to the absence of a comprehensive guide describing how to achieve integrated hydrological and hydrogeological models. Compared to measured groundwater levels in boreholes, the simulated groundwater levels in the bedrock were too high in the Surface system groundwater flow model (Bosson et al. 2008), whereas the simulated groundwater levels in the regolith were too high in the Bedrock system groundwater flow model (Follin et al. 2007b). Besides the absence of a guide requiring hydrological and hydrogeological integration, the characteristic, but complex, structural-hydraulic conditions observed in the uppermost part of the bedrock were postulated to affect the hydraulic interaction between the Surface system and the Bedrock system (cf. Figure 1-3). All in all, the lessons learned in SDM-Site are key for this methodology report and the design of the proposed modelling protocol.

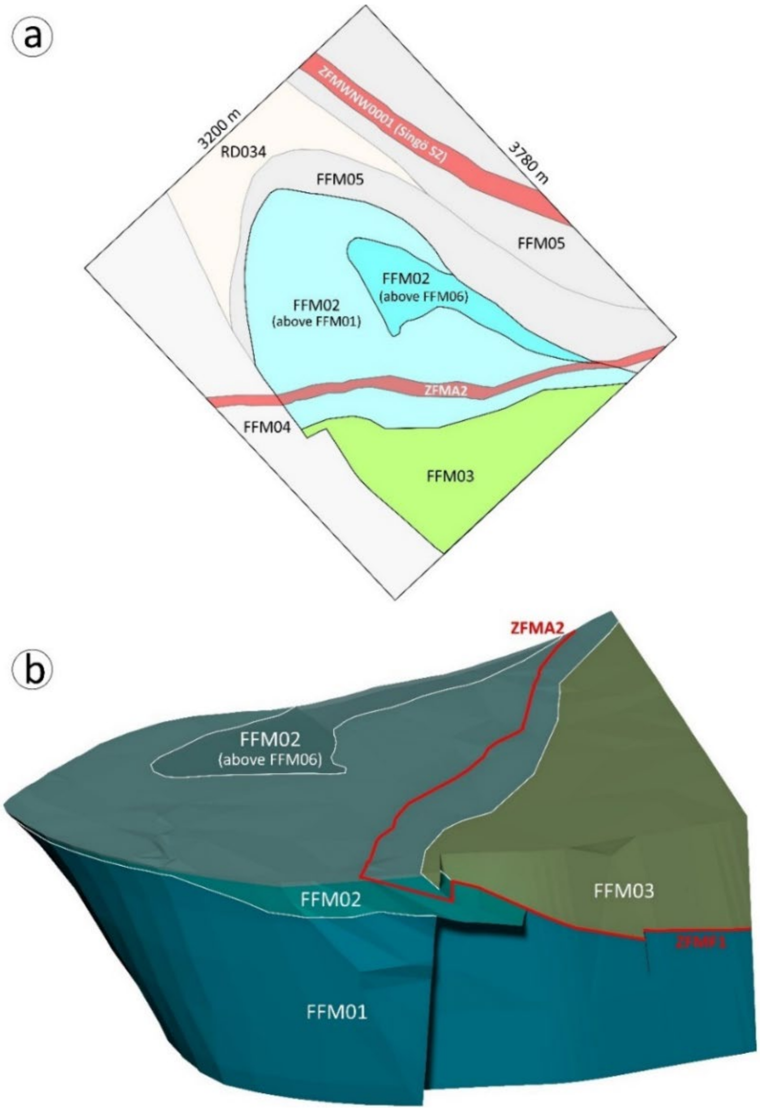

Figure 1-2. *a) Top view of the fracture domain model (FFMxx) inside the SDM-Site local model domain. Volumetric representations of deformation zones ZFMA2 and ZFMWNW0001 (Singö DZ) are shown as references; they are not part of the fracture domain model. (b) Oblique view towards ENE of the 3D model for fracture domains FFM01, FFM02 and FFM03 inside the SDM-Site local model domain. FFM06 is enclosed by FFM01 and situated beneath FFM02 and is for this reason not visible. Outcropping trace of the gently dipping deformation zone ZFMA2 is shown in red as a reference. The rock masses above and below ZFMA2 are named hanging wall and footwall, respectively. The bottom of the fracture domain model is located at –1,100 m. From Peterson et al. (2024).*

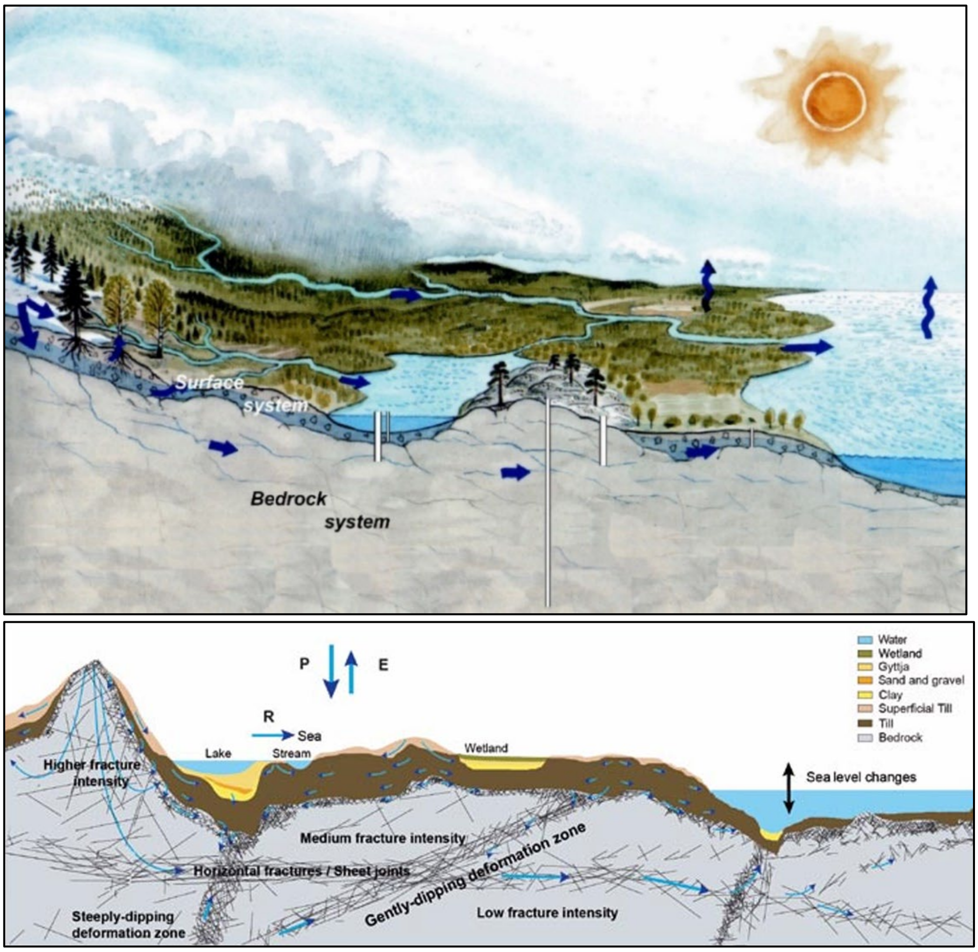

Figure 1-3. *Top: Illustration of the earthbound parts of the hydrologic cycle. Monitored groundwater levels in boreholes were modelled with system-specific flow modelling tools, one for the Surface system and another for the Bedrock system. Bottom: Illustration of the intensely fractured near-surface bedrock in Forsmark and its conceived effect on the hydraulic interaction between the flows in the Surface system and in the Bedrock system, respectively. Recharge from above and discharge from below flow laterally towards the sea. P=precipitation, E=evapotranspiration, R=runoff. Reproduced from Follin et al. (2007b).*

1.4 Data for future modelling

Regarding data for future integrated hydrological and hydrogeological modelling, new boreholes will be drilled from excavated underground openings to characterize the geometric and material properties of the bedrock adjacent to the openings at different depths. These data are key for the concepts considered by SKB for future DFN modelling described in the separate methodology report for DFN modelling (Selroos et al. 2022).

No new boreholes are planned to be drilled from the ground surface, except in the uppermost bedrock near the planned accesses. However, these boreholes are not intended for geoscientific investigations but for curtain grouting to a depth of approximately 60 m. It is noted that grouting will also be used, when needed, in the short boreholes drilled into the bedrock ahead of the tunnel front to control groundwater inflow. The aspects listed above imply that existing data from past investigations in boreholes drilled from the ground surface will remain key also for future hydrological and hydrogeological flow modelling.

1.5 Report structure

Chapter 1 describes the background and objectives of this methodology report.

Chapter 2 reviews SKB's system approach for hydrological-hydrogeological modelling, including: conceptual models for the discretely fractured Bedrock system and the porous Surface system (regolith), handling of hydrological processes, and assignment of hydraulic boundary and initial conditions.

Chapter 3 revisits characteristic structural-hydraulic observations within the local model domain (Figure 1-2). Particularly, the extensive hydraulic interferences in the uppermost c. 150 m of the bedrock, the hydraulic resistance for flow transverse the regional Singö deformation zone, and the strong decrease with depth of the linear intensity of open and flowing open fractures below c.150 m depth.

Chapter 4 presents the proposed protocol for integrated hydrological and hydrogeological modelling. The protocol strives for consistent performance between the modelling tools intended for Surface system flow modelling and Bedrock system flow modelling, respectively. Chapter 4 describes the workflow, present-day flow modelling tools, and the methods in which discrete fracture network (DFN) model realisations are transformed into "equivalent continuous porous medium" (ECPM) model realisations. The underpinning strategy of the protocol is that discrete and porous media flow modelling tools must have at least one calibration target in common and that the calibration result(s) must be sufficiently consistent to ensure confidence regarding their usage in other applications.

1.6 Limitations

First, though DFN modelling is a cornerstone for the proposed protocol for integrated hydrological and hydrogeological modelling, this methodology report does not deal with DFN modelling per se. To appreciate the implications of the proposed protocol for DFN modelling, the reader is recommended to also read Selroos et al. (2022), who describe the DFN concepts considered by SKB for future DFN modelling, calibration, and validation. Notably, both historic concepts and more novel ones, including structural conditioning and hydromechanical calibration, are described in Selroos et al. (2022).

Second, it is stated in Section 1.3 that the modelling protocol focuses on the hydraulic interaction between the earthbound flows of the hydrologic cycle inside the local model domain. This simply reflects the abundance of surface-based boreholes, investigations, and data. The usage of data outside the local model domain for structural conditioning and hydraulic calibration is more uncertain.

Third, this methodology report intends to support future needs for integrated site-descriptive hydrological and hydrogeological modelling. However, pending the acquisition of new data, which will not commence before the constructions of accesses starts, the protocol for integrated hydrological and hydrogeological modelling is limited to handle the surface-based data acquired in SDM-Site (SKB, 2008) and Baseline Forsmark (2025).

Fourth, while the design of the proposed protocol is independent of the specific modelling tools used, the tools discussed in Chapter 4, along with the modelling protocol itself, have been used by SKB for nearly 20 years, some of which may continue to play a central role in the future. However, at the time of writing this methodology report, it is not decided which tools will be used in the future.

2 SKB's systems approach

2.1 Hydrology versus hydrogeology

The term hydrology usually refers to all components of the hydrologic cycle, i.e. water flows and storages of atmospheric, surface and subsurface waters. Here, the term hydrology is specifically used for the occurrence and flow and storage of surface water (lakes, ponds, streams and sea basins). The term hydrogeology is specifically used for the occurrence, flow and storage of water below the ground surface, particularly in the saturated zones of the regolith and the bedrock. Differences in processes, time scales, geometries, and properties motivate a division of earthbound flows of the hydrologic cycle into two parts, a Surface system and a Bedrock system (Figure 2-1).

2.2 Surface system versus Bedrock system

The Surface system modelling considers three flow domains, one hydrological and two hydrogeological. The hydrological flow domain consists of lakes, ponds, streams and sea basins. The hydrogeological flow domains represent the regolith and bedrock. The regolith is modelled as a stratified porous medium made up of several units each having calibrated characteristic hydraulic properties. Though the fractured bedrock below the regolith is a discrete medium, it is also treated as a porous medium in the Surface system modelling. In summary, the models of the hydrological flow domain and the regolith are both deterministic models, whereas the bedrock model is stochastic. The equivalent hydraulic properties of the fractured bedrock are derived by means of upscaling.

The Bedrock system considers two hydrogeological flow domains, the bedrock and the regolith, with hydrology modelled only through definition of surface boundary conditions. Surface runoff is not considered. The bedrock consists of two main classes of discrete fractures, where the deformation zones being deterministic and distinct individual domains of higher fracture frequency than the fracture domains although some can be single discontinuities (breaks) of millimetre scale thickness. Different types of discrete fractures are modelled stochastically within the rock mass of the fracture domains, including so-called possible deformation zones and sheet joints that may both be partly conditioned to data. The sheet joints are considered vital for the interaction between the Bedrock system and the Surface system and their inclusion in the methodology reports (Follin 2008, Selroos et al. 2022) is a significant amendment to the generic modelling approach by Rhén et al. (2003).

A key objective of the Surface system flow modelling is to establish a credible flow model of the surface and near-surface conditions prior to start of constructions that can be used to clarify whether observed variations in groundwater levels, lake levels and runoff rates during constructions are caused by natural meteorological/hydrological changes or due to anthropogenic changes following various engineering activities, e.g. changes in landscape morphology and water courses, bedrock excavations and grouting. To meet this objective, the calibration of the Surface system modelling uses long time series of monitored state variables. The calibration requires that the monitoring is made on a diurnal basis.

A key objective of Bedrock system flow modelling is to develop a credible model suitable for predicting post-closure groundwater flow and solute transport following repository closure and full saturation (hydraulic recovery). Here, 'long-term' refers to the entire assessment timescale, including freezing and ice loading effects. In the hydrogeological modelling for SR-Site, the end of the so-called temperate period was set at 12 000 AD (SKB 2011). However, when assessing groundwater composition, even longer timescales need to be considered. Due to its discrete nature and strong spatial variability, the hydraulic calibration of Bedrock system modelling requires conditioned stochastic discrete fracture network (DFN) realisations. That said, it is noted that the concepts intended for future DFN modelling applications are not described here but in the methodology report by Selroos et al. (2022), see Table 1-1.

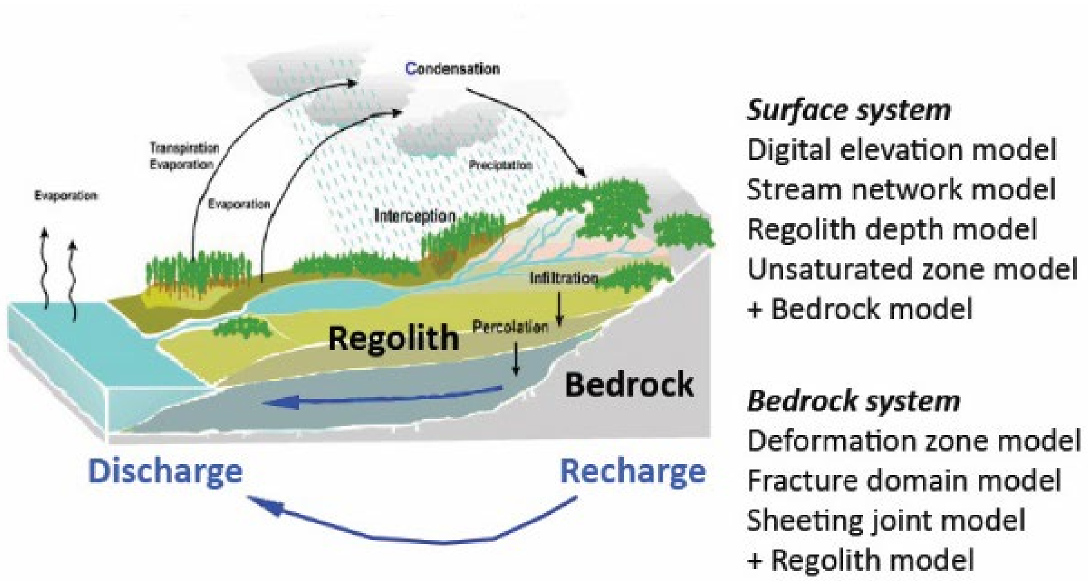

Figure 2-1. *Schematic of the hydrologic cycle, regolith and bedrock. Differences in processes, time scales, geometries, and properties motivate a division of earthbound part of the hydrologic cycle into two parts, a Surface system and a Bedrock system.*

2.3 Main reports related to hydrology and hydrogeology

Table 2-1 and Table 2-2 present the main reports related to hydrology and bedrock hydrogeology, respectively, produced as part of the previous modelling and investigation stages (SDM-Site, SDM-PSU, and the SFK access area update), and those of the current Baseline Forsmark modelling stage (SKB 2025). It is noted that the table only shows main reports; these are based on a large number of other reports regarding hydrological investigations and monitoring.

Table 2-1. Main reports related to hydrology, produced as part of SDM-Site, SDM-PSU, the SFK access area update, and those of the current Baseline Forsmark modelling stage. The listed reports number are accessed by visiting https://skb.se/publikationer/

	SDM-Site	SDM-PSU	SFK access area	Baseline Forsmark
Data reports – properties	R-08-08	R-13-19	P-17-19	R-22-07
Data reports – state variables	R-08-10	R-13-20	P-17-19	R-24-03
Conceptual and quantitative water flow modelling	R-08-09, R-08-10	R-13-19	-	R-23-06
Surface system synthesis	R-08-11	TR-14-06	-	-
Main report	TR-08-05	TR-11-04	R-17-13	R-24-01

Table 2-2. Main reports related to bedrock hydrogeology, produced as part of SDM-Site, SDM-PSU, the SFK access area update, and those of the current Baseline Forsmark modelling stage. The listed reports number are accessed by visiting https://skb.se/publikationer/

	SDM-Site	SDM-PSU	SFK access area	Baseline Forsmark
Data reports – properties	R-07-48	R-11-03	P-16-27, P-17-17	R-22-07
Data reports – state variables	R-08-10	-	P-17-19	R-24-03
Conceptual and quantitative groundwater flow modelling	R-07-49, R-08-23	R-11-10	-	R-23-06
Bedrock system synthesis	R-08-95	R-13-25	-	-
Main report	TR-08-05	TR-11-04	R-17-13	R-24-01

2.4 Bedrock system

2.4.1 Conceptual model for flow and solute transport

Figure 2-2 shows a conceptual framework for discrete fractures of different types and scales in crystalline rock. SKB's conceptual model for groundwater flow and solute transport in fractured crystalline rock is that solutes are transported by the advection in the flowing (mobile) water in the permeable openings of connected discrete fractures. At the same time, sorption onto the minerals on fracture surfaces and the adjoining rock matrix via molecular diffusion through porewater are significant physical retardation mechanisms for migration and the evolution of groundwater composition. Without the retention implied by sorption and the diffusion between the mobile fracture water and the immobile (stagnant) water in the rock matrix (rock matrix diffusion, RMD), hydrogeological models will not be able to reproduce the hydrogeochemical evolution and measured data correctly. For example, transport of dilute water from surface to depth will not be correctly described without the incorporation of RMD. Further, salt transport in flowing fractures gives rise to variations in groundwater salinity and hence fluid density. The fluid density is also affected by temperature differences. The density variations create density-driven flows. These flows are accounted for in the flow modelling by considering buoyancy effects in the mass balance equation.

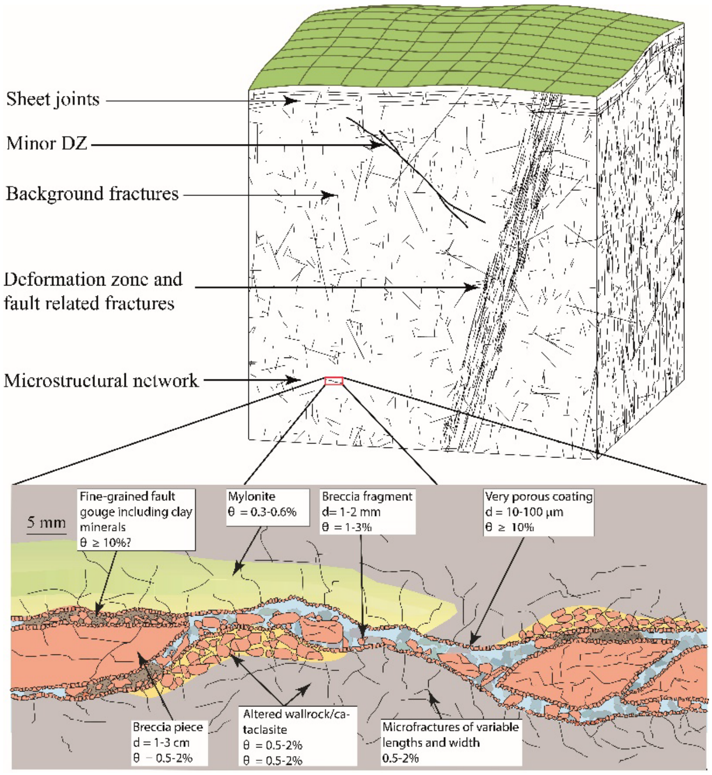

Figure 2-2. *Conceptual framework for fractures of different types and scales in sparsely fractured rock. The insert at the bottom shows a highly magnified schematic of fractures at the microstructural scale after Winberg et al. (2003), which can be down to the scale of the micro-fissures between individual grains.*

2.4.2 Concepts for discrete fracture network modelling

Follin (2008) describes the methodology for *hydrogeological* DFN modelling that was used in SDM-Site and SR-Site. Below, this methodology is referred to as DFN-2008. Selroos et al. (2020) presents an interdisciplinary methodology suitable for *all kinds* of DFN models within site descriptive modelling, construction of final disposal facilities, and analysis of post-closure safety. The interdisciplinary methodology integrates the basic DFN concepts developed in SDM-Site for geological DFN modelling (Fox et al. 2007) and DFN-2008 with new ones. Examples of such new concepts are hydromechanical coupling, genetic fracture generation including growing fractures, heterogeneous description of individual fracture planes, deformation zones consisting of multiple discrete fractures, and a framework for handling conceptual uncertainties at different stages. Below, this interdisciplinary methodology is referred to as DFN-2020. It is noted that several DFN-2008 concepts are integrated into DFN-2020.

The focus of DFN-2008 (Follin 2008) is on the linear intensity of open fractures modelled as regularly shaped planar surfaces (squares, disks etcetera) using statistically driven models with one set of generation parameters ('model recipe') for each fracture set and fracture domain. The generation of single, open fractures is assumed to follow a Poisson process and a power-law size-intensity model. Another key assumption is that the connectivity and transmissivity of open fractures can be mimicked by means of calibrated flow simulations using PFL data, see Figure 2-3. Finally, large deformation zones are modelled as undulating triangulated surfaces to account for the observed depth trend and lateral spatial variability of the in-plane transmissivities evaluated from hydraulic tests in boreholes. A key feature of DFN-2020 (Selroos et al. 2022) is growing planar objects of irregular shapes (non-symmetric polygons) using geologically driven DFN models, where structural elements from the deterministic geological model are used to constrain variations in fracture intensity and size, see Figure 2-4. A crucial part in hydrogeological applications of DFN-2020 is the hydro-mechanical determination of openness.

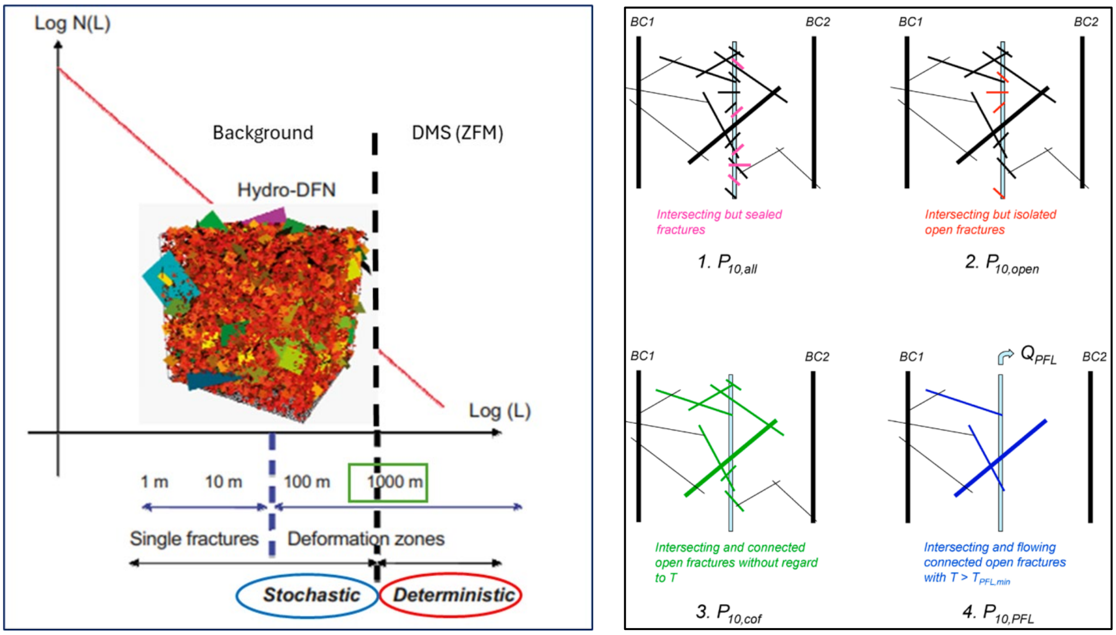

Figure 2-3. *Left: Illustration of the DFN-2008 concept showing a single power-law frequency model for open fractures on all scales ("tectonic continuum"). Right: Illustration of the relations between all fractures, open fractures, connected open fractures, COF, and PFL data in a borehole: P10,all ≥ P10,open ≥ P10,cof ≥ P10,pfl. From Follin (2008). From Follin (2008).*

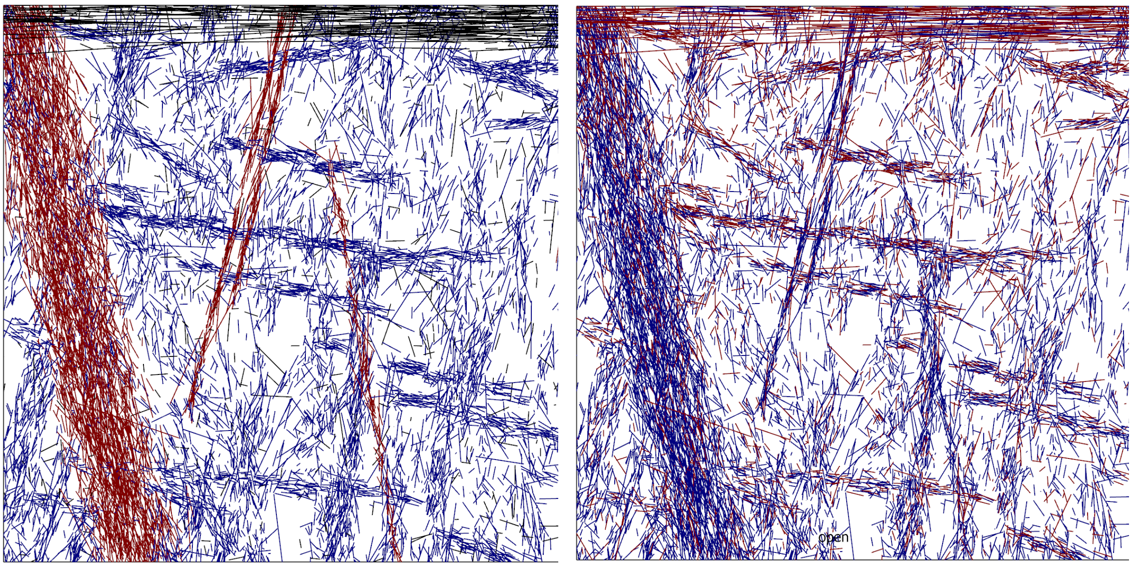

Figure 2-4. *Illustration showing the geologically driven DFN-2020 concept. Note that deformation zones, both deterministic and stochastic, are also modelled as discrete fracture networks. From WSP (Simon Libby, pers. comm. 2023).*

2.5 Surface system

2.5.1 Conceptual model

Figure 2-5 shows the conceptual stratigraphical model for the regolith in Forsmark (Petrone et al. 2020). The model shows in what order the regolith layers ('z layers') are distributed in different environments. However, at a particular location, e.g., a till-dominated recharge area, some of the layers might be missing even though the layers always are distributed in the order shown in Figure 2-5.

2.5.2 Regolith depth and stratigraphy model

The conceptual stratigraphical model has been used together with the digital elevation model (DEM), a map of the surface distribution of regolith, and more than one hundred borehole soundings to construct a regolith depth and stratigraphy model (RDM). The RDM is a deterministic representation in 3D of the spatial distribution and thickness of the nine most commonly occurring regolith types in the Forsmark catchment (Figure 1-1). The horizontal resolution of the RDM is 20 m by 20 m and the hydraulic parameterisation is based on the inferred properties from single-hole tests in groundwater-monitoring wells and sieve analyses (Earon et al. 2025), and results from previous Surface system modelling studies (Table 2-1).

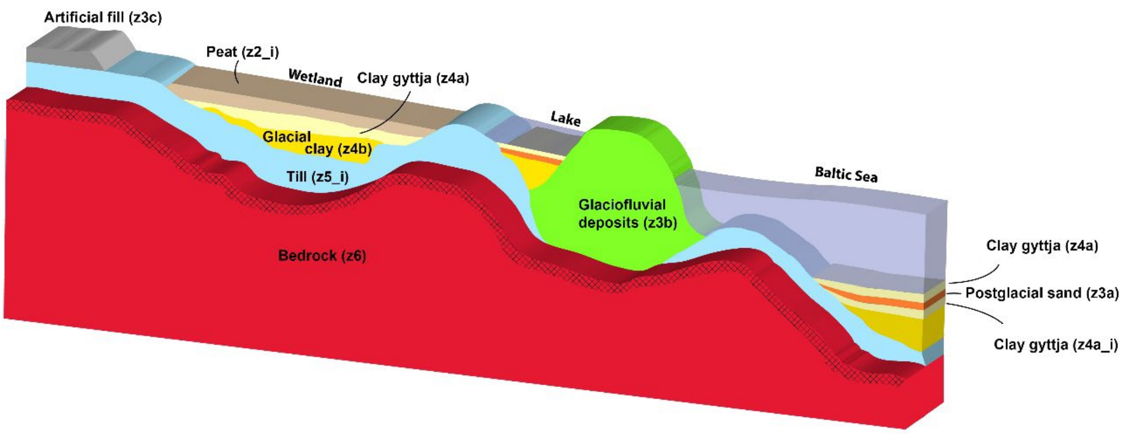

Figure 2-5. *The general distribution of the regolith layers ('z layers') used in the RDM. From Petrone et al. (2020).*

2.6 Hydrological processes

Figure 2-6 illustrates a conceptual holistic hydrological and hydrogeological model for both natural and anthropogenic processes. Below, the main components and associated natural processes of the hydrologic cycle are briefly described. Atmospheric, surface and near-surface processes are weather (and season) dependent and hence modelled on a diurnal basis in the Surface system flow modelling. Pseudo steady state flow is generally assumed in the Bedrock system flow and transport modelling as the effects of diurnal changes in surface and near-surface processes typically decrease with depth. Long-time averages (over several years) might then be used as a proxy. Below, the acronyms SS and BS are used to clarify where each process is handled.

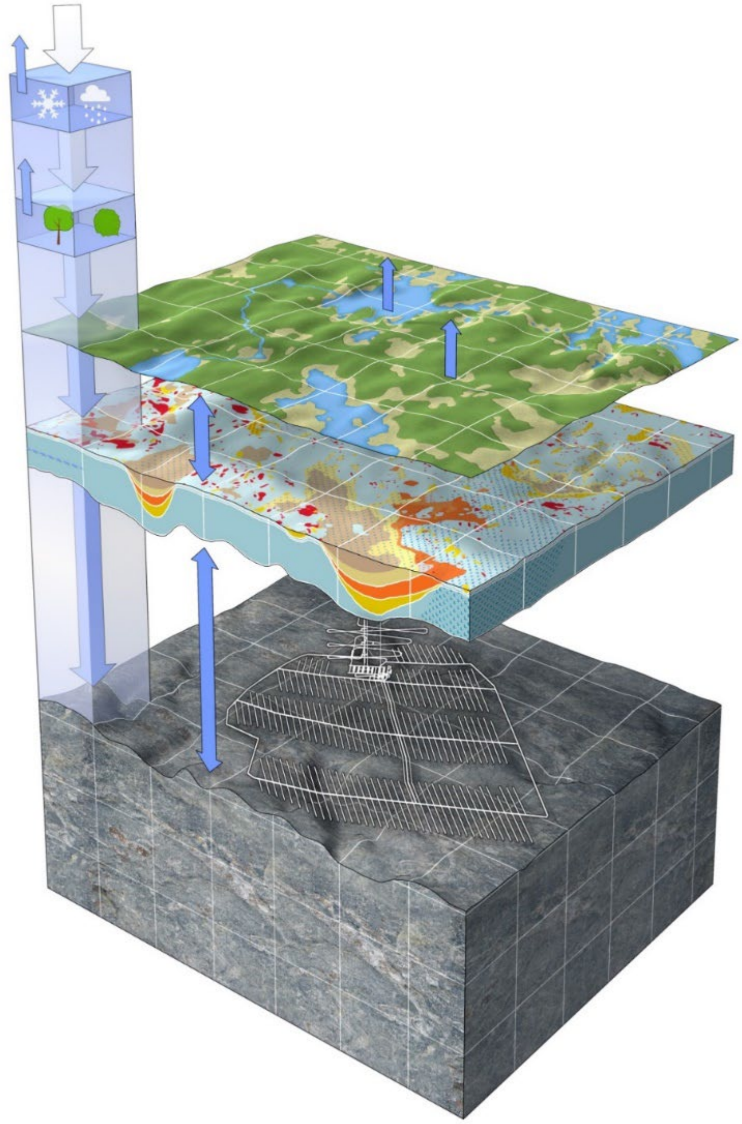

Figure 2-6. Oblique view of an integrated conceptual hydrological and hydrogeological model that handles both natural and anthropogenic processes. From the top: Vegetation and land use, regolith, stream network and other waters in the Surface system, and the Bedrock system, including a hypothetical layout of SFK including its accesses. From Johansson (2019).

The atmosphere (SS): The main processes of the atmospheric component are precipitation (actual rainfall and snow accumulation), snow melt and ET (actual evapotranspiration). The size of ET (interception, evaporation from ponded water, transpiration and soil evaporation) and its spatial and temporal variations depend on the meteorological conditions, and interactions with other components, such as amounts of available water (water in regolith and surface water), and vegetation as a driver for transpiration.

Vegetation and land use (SS): Vegetation and land use influence ET, which in turn influences infiltration, groundwater recharge, unsaturated water flow and saturated groundwater flow. Conceptual and quantitative models must therefore include spatially and temporally variable vegetation- and land-use specific parameters that govern interception, evaporation and transpiration.

Water in regolith (SS): The regolith component receives water from and loses water to the ground surface, surface waters and the atmosphere, and it also interacts with water in the underlying bedrock. Saturated groundwater flow should be modelled in 3D, whereas modelling of water flow in the unsaturated zone as a 1D (vertical) process is generally appropriate due to the near-surface groundwater table. The present-day climatic conditions at Forsmark implies that ground frost is an important process in conceptual and quantitative models.

Water in bedrock (SS and BS): The bedrock component interacts with water in the overlying regolith, and it also receives water from and loses water to the ground surface, surface waters and the atmosphere (in bedrock outcrop areas). Saturated groundwater flow should be modelled in 3D because of the complexity of the geological structural model, whereas modelling of water flow in the unsaturated zone should be modelled as 1D (vertical) or as a 3D process depending on the depth of the unsaturated zone in the bedrock.

Surface water (SS): The surface-water component represents water in lakes, ponds, streams and the sea, and requires geometrical descriptions including topography and bathymetry. This component receives water from and loses water to the atmosphere, and its interactions with the regolith and bedrock require conceptual and quantitative models to include spatially variable flow-resistance parameters. The geometry of the stream network must be described deterministically as it interacts both with other surface waters and with the regolith and bedrock components. Moreover, the near-coastal location of Forsmark implies that the sea level variations constitute a transient hydrological boundary condition. This boundary condition influences the process of submarine groundwater discharge, and it may also cause sea-water transgression into near-coastal lakes and flooding of land areas. The present-day climatic conditions at Forsmark implies that ice coverage is an important process in conceptual and quantitative flow models.

Saline water (BS): Figure 2-7 shows observations of groundwater salinity (TDS, g/L) and temperature (°C) with depth down to −1,000 m elevation in several surface-drilled boreholes at Forsmark. The data suggest a water density of approximately 1000.7 kg/m^3 near ground surface, 1007.4 kg/m^3 at −500m elevation and approximately 1010.0 kg/m^3 at -1,000 m elevation (CSGNetwork, 2025). The density at greater depths than 1000 m is unknown but potentially it is higher given the trends in salinity data acquired at Laxemar (SKB 2009) and at Olkiluoto (Posiva 2009). Accounting for density-driven flow is essential for the Bedrock system flow and solute transport modelling at Forsmark, because of its effects on hydraulic pressure gradients and the measured pressure heads at depth. For example, changes in water density during Holocene time occur in response to the rebound of the lithosphere and marine transgression. This phenomenon was modelled as part of paleoclimatic simulations used for evaluating the liability of the stochastic structural-hydraulic description (Follin et al. 2007b, 2008) in SDM-Site. Salinity and density-driven groundwater flow was not considered in the Surface system flow modelling in SDM-Site, which assumed that all types of groundwater could be modelled as fresh water (Bosson et al. 2008). This simplification is acceptable provided that the salinity of water is less than 1 % (Anderson et al. 2015), which is the case down to approximately −500 m elevation according to Figure 2-7a.

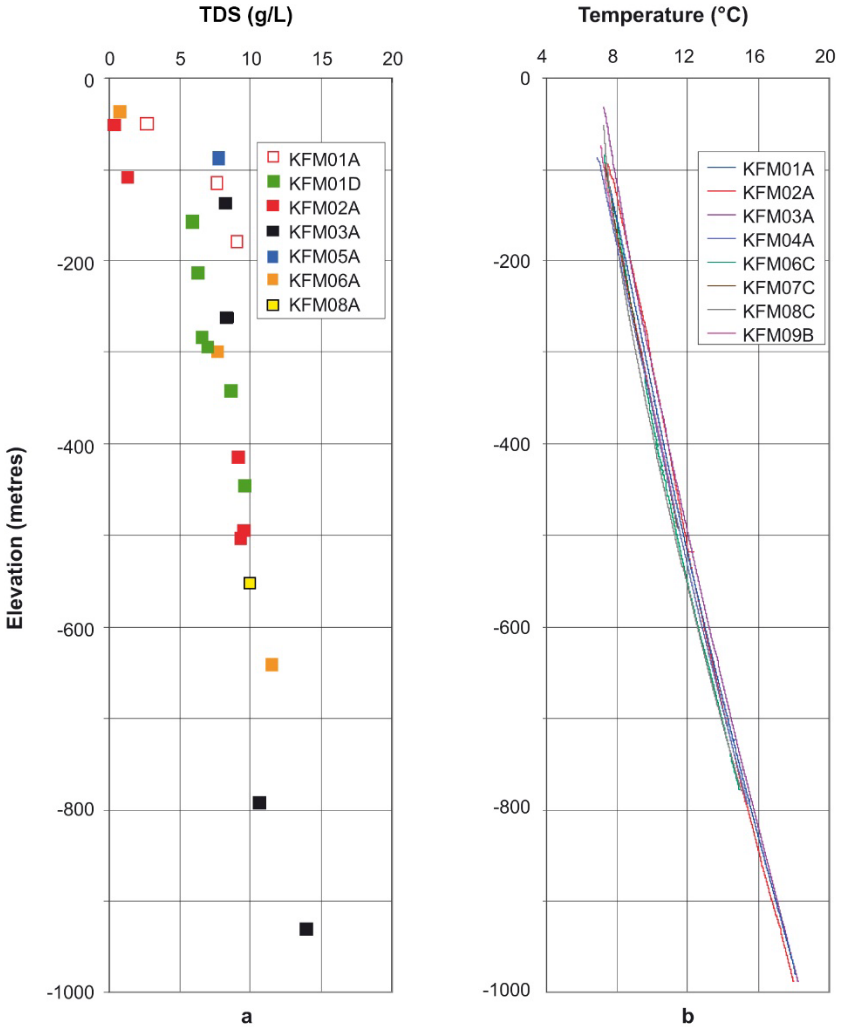

***Figure 2-7.** Present-day content of total dissolved solids (TDS) and temperature for seven (a) and eight (b) cored boreholes in Forsmark, respectively. Salinity and temperature both affect the groundwater density. From in Follin (2008).*

Paleoclimatic evolution (BS): Figure 2-8 illustrates the paleoclimatic evolution of the Forsmark area from the latest deglaciation to the present. The relative sea level (RSL) is defined as the height of the contact between the ocean surface and land. A rise in the RSL can be caused by an increased elevation of the ocean surface or a decreased elevation of the land surface, for example due to ice loading. In the Forsmark area, there has been a rebound of the lithosphere since the Last Glacial Maximum (LGM) and a rising ocean sea level during the same period. However, the positive glacial isostatic adjustment (causing the land area to expand) has been stronger than the eustatic rise (process causing the sea area to expand); thus, the RSL has decreased, and new land has developed since LGM. The evolution shown in Figure 2-8 was handled in the Bedrock system flow modelling for SDM-Site in matching against observed hydrogeochemical profiles in deep boreholes. Follin et al. (2007b, 2008) note, however, that the associated model parameters and conditions are mainly transport related and not involved in the calibration against other groundwater flow targets such as cross-hole pumping tests and natural groundwater levels in the regolith and the shallow bedrock domain. The modelling of the paleoclimatic evolution in the Bedrock system flow modelling in SDM-Site is commented in Section 2.7.2 and in Chapter 5.

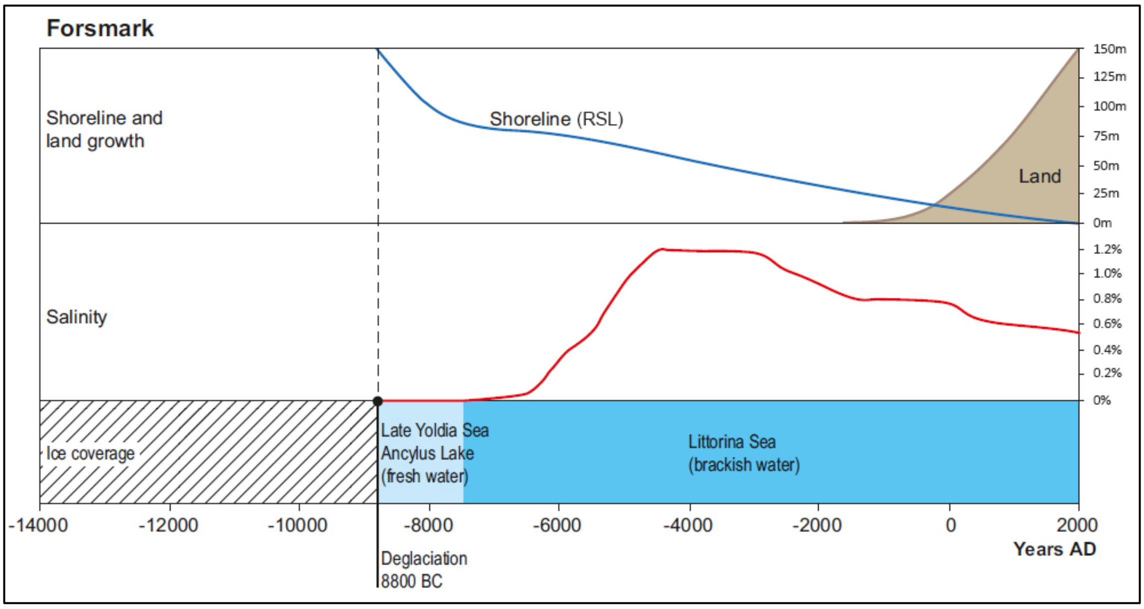

Figure 2-8. *Composite illustration of the paleoclimatic evolution of the Forsmark area from the latest deglaciation to the present. The blue curve shows the elevation of the shoreline (expressed as relative sea level, RSL), the red curve shows variations in salinity of the open Bothnian Sea offshore from Forsmark and the brown area represents the successively increasing rebound. From Söderbäck (ed) (2008).*

2.7 Hydraulic boundary and initial conditions

2.7.1 Boundary conditions

The choice of boundary condition depends on the location of the boundary and the conditions related to the problem/system under study, see Table 2-2, Table 2-3, and Table 2-4. The most common boundary conditions for flow and one for transport are:

A. Dirichlet (first kind) flow boundary condition: Specified head boundary.

B. Neumann (second kind) flow boundary condition: Specified flux boundary.

C. Cauchy (third kind) flow boundary condition: Head-dependent flux boundary.

D. Dirichlet (first kind) solute boundary condition: Specified concentration boundary.

A Cauchy (or mixed) boundary condition for head is often used for complex outflow and inflow conditions, including flux exchange between groundwater and surface water. Further, a mixed concentration and outflow condition is often used for solute transport.

Table 2-1. Parameters for the top boundary conditions

Parameter	Notation	Unit	Spatial representation	Comment
Precipitation	P	mm/y, mm/d	Constant or variable over time. Spatial distribution if required.	
Potential evapotranspiration	PET	mm/y, mm/d	Constant or variable over time. Spatial distribution if required.	
Surface water and sea level	H	M	Constant or variable over time.	
Salinity	TDS	mg/L	Constant or variable over time.	Salinity of meteoric, lacustrine and marine waters.
Runoff	Q_R	m^3/s	Constant or variable over time.	Runoff rates are estimated or measured for larger catchment areas.
Pumping rate	Q_P	m^3/s	Constant, variable over time or Cauchy (e.g. you inject until a certain bottom hole pressure is achieved).	
Infiltration rate	Q_I	m^3/s	Constant or variable over time and space.	

Table 2-2. Parameters for vertical and bottom boundary conditions

Parameter	Notation	Unit	Spatial representation	Comment
Pressure	p	kPa	Constant or variable over time.	Difficult to assess more exactly from measurements.
Salinity	TDS	mg/L	Constant or variable over time.	Difficult to assess more exactly from measurements.
Flux	q	$m^3/m^2/s$	Often assumed to be no flow.	A model parameter.

Table 2-3. Parameters for open repository boundary conditions

Parameter	Notation	Unit	Spatial representation	Comment
Pressure	p	kPa	Constant	Atmospheric pressure in underground openings. Skin properties are required to have sensible inflows, allowing for shotcrete and hoop stress etc.
Flux	q	$m^3/m^2/s$	Constant or variable over time and space	Relaxes the need for using skin properties.

2.7.2 Initial conditions

Initial conditions are required for transient simulations. If the modelling task is to simulate the transient evolution of a single-hole or cross-hole (interference) test, a stationary simulation of the undisturbed state of flow prior to testing might be adequate as initial conditions. Such a stationary simulation should ideally be based on a previously calibrated groundwater flow model. If the modelling task involves detection of anthropogenic hydrologic disturbances, several years of time series simulations might be used to reduce the effect of seasonal and annual fluctuations in water storage (Bosson et al. 2008, 2010).

If the modelling task involves simulation of variable-density flow over longer times, e.g., transient simulation of the paleoclimatic evolution during Holocene time, initial hydrogeochemical conditions are required of the spatial distribution of main chemical constituents and so-called reference waters (water types) in the mobile (advective) water in the fracture system as well as the immobile (diffusive) water in the rock matrix (Laaksoharju et al. 2008). As the actual setting of these conditions are uncertain, the initiation needs to be defined in corporation with the hydrogeochemical modelling to assure conceptual consistency between disciplines, see Mercier et al. (2025).

The initial conditions used in SDM-Site and SR-Site are shown in Figure 2-9 and may serve as an introduction in this regard (Follin et al. 2007b, 2008; Joyce et al. 2010; Vidstrand et al. 2010; Follin and Hartley 2014; Joyce et al. 2014; Vidstrand et al. 2014). The chemical compositions of the reference waters depicted in Figure 2-9 are summarised in Table 2-4. In the hydrogeological model, the transport of solutes was modelled in terms of the infiltration and mixing of several different reference waters that were assumed to be transported conservatively, i.e. without reaction, but subject to advection, dispersion, and diffusion in both the fracture water and the porewater (i.e. rock matrix diffusion). The paleoclimatic simulations were started at 8000 BC and the development of the hydrochemistry was calculated according to the changes in sea level azimuth and salinity shown in Figure 2-8. The chemical compositions of the reference waters were fixed in time. Therefore, given the simulated mixture of references waters (defined by the mass fraction) at any point in space and time, the concentrations of the major ions or environmental isotopes were calculated by multiplying the reference water fraction by the concentration of the component in that reference water and then summing over the reference waters. Finally, the predicted concentrations, or isotope ratios, were compared with the measured data.

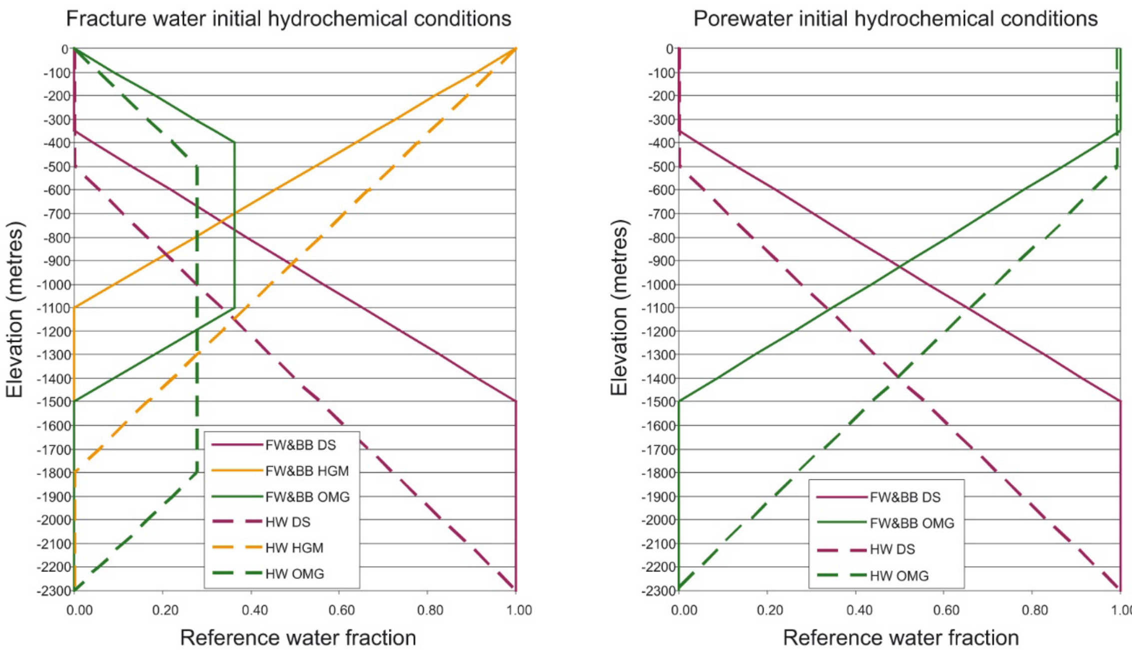

Figure 2-9. *Assumed initial hydrogeochemical conditions at 8000 BC in SDM-Site (Follin 2008). DS = Deep Saline Water, HGM = Holocene Glacial Melt Water, OMG = Old Meteoric-Glacial Waters. Different profiles were assumed for the footwall (FW) and bordering bedrock (BB) regions of the gently dipping deformation zone ZFMA2 compared to the hanging wall (HW) bedrock region of this zone, see Follin (2008) for an explanation of these bedrock regions. From Follin (2008).*

Table 2-4. Compilation of reference water compositions for Forsmark. Modified after Laaksoharju et al. (2008)

Reference Water	Na mg/L	K mg/L	Ca mg/L	Mg mg/L	HCO_3 mg/L	Cl mg/L	SO_4 mg/L	Br mg/L	δ^2H o/oo SMOW	$\delta^{18}O$ o/oo SMOW
Deep Saline (DS)	8,200	45.5	19,300	2.12	14.1	47,200	10	323	-44.9	-8.9
Holocene Glacial Melt Water (HGM)	0.17	0.4	0.18	0.1	0.12	0.5	0.5	0	-158	-21
Littoria Sea Water (LS)	3,674	134	151	448	92.5	6,500	890	22.2	-37.8	-4.7
Present-day Meteroric Water (PM)	274	5.6	41.1	7.5	466	181	85.1	0.6	-80.6	-11.1

3 Key structural-hydraulic observations

A robust conceptual understanding of the structural and hydraulic observations within the local model domain shown in Figure 1-2 is essential to the development of the site-specific protocol presented in this methodology report. Ten essential observations underpinning the protocol are listed in Table 3-1 and Table 3-2, six of which are also shown in Figure 3-1 through Figure 3-8. The ten observations can be divided into three categories:

- Hydraulic interferences in the uppermost c. 150 m of bedrock.
- Hydraulic resistance for flow transverse the regional Singö deformation zone.
- Linear intensity and transmissivity of open fractures.

These ten conditions influence our conceptual understanding of surface-based investigations of the Forsmark site, flow model calibrations, and predictive simulations, including: the spatial distribution of groundwater inflow (recharge) and outflow (discharge) areas, prediction of water table drawdowns during the construction of repository accesses, vertical groundwater fluxes between the ground surface and repository depth, and simulations of particle tracking exit locations.

Table 3-1. Significant observations in SDM-Site

ID	Observation
1	Large subhorizontal fractures/sheet joints with distinct apertures in the uppermost part of the bedrock along the inlet channel of seawater to the nuclear power plant (Follin 2007b).
2	Exceptionally high yields of water in percussion (drilled) boreholes. The median yield of the first 22 percussion boreholes drilled into the uppermost c. 150m of bedrock within the local domain is c. 12,000L/h. This value is c. 20 times higher than the median yield of the domestic water wells drilled elsewhere, both outside the local domain (Gentzschein et al. 2007) and in Sweden in general according to the archive of wells hosted by the Geological Survey of Sweden (Berggren 1998).
3	The uniform (identical) groundwater levels (total hydraulic heads) measured in the percussion boreholes drilled into the uppermost c. 150m of bedrock within the local model domain. The value of the uniform groundwater level is c. +0.5m above the sea level. In contrast, the average groundwater level measured in the percussion boreholes drilled outside the local model domain is c. +2.8m above the sea level (Follin et al. 2008). This difference implies that the fractures in the uppermost bedrock within the local model domain function hydraulically as interconnected vessels.
4	The average groundwater levels in the groundwater-monitoring wells installed in the regolith within the SDM-Site local domain is c. +0.8m above the sea level. In contrast, the average groundwater level measured in the groundwater-monitoring wells installed in the regolith outside the local domain is c. +3.5m above the sea level (Follin et al. 2008). This difference reinforces the observation in #3.
5	The extensive and rapid transmission of hydraulic responses during the cross-hole (interference) pumping test that was run over three weeks during the summer of year 2006 in percussion borehole HFM14. HFM14 is drilled in the centre of the local model domain (Gokall-Norman and Ludvigson 2008a, Follin et al. 2007b). Notably, a second cross-hole test in HFM14 was run in 2007 with identical outcome (Gokall-Norman and Ludvigson 2008b, Follin et al. 2008).
6	The extensive and rapid transmission of hydraulic responses during the cross-hole pumping test that was run over two weeks during the summer of year 2007 in percussion borehole HFM33. HFM33 is located south of the Singö deformation zone within the local domain, c. 2km north of HFM14 (Gokall-Norman and Ludvigson 2008b, Follin et al. 2008).
7	The lack of hydraulic responses in nearby boreholes drilled through the Singö deformation zone or into the bedrock on the northern side of this zone during the cross-hole test that was run over two weeks during the summer of year 2007 in percussion borehole HFM33, cf. above (Gokall-Norman and Ludvigson 2008b, Follin et al. 2008).

Table 3-2. Significant observations posterior to SDM-Site

ID	Observation
8	The extensive and rapid transmission of hydraulic responses during the cross-hole pumping test that was run over three weeks during the summer of year 2018 in percussion borehole HFM43. HFM43 in located close to the planned SFK access area within the local domain, c. 1km northwest of HFM14 (Föhlinger et al. 2020).
9	The lack of hydraulic responses in the additional boreholes drilled into the Singö deformation zone or into the bedrock on the northern side of this zone during the cross-hole test that was run over two weeks during the fall of year 2018 in percussion borehole HFM33 located south of the zone (cf. above) (Föhlinger et al. 2020).
10	The high frequency of subhorizontal open fractures, including sheet joints with distinct apertures, in fourteen cored boreholes (KFM13-23, 25-27) drilled to c. 100m depth into fracture domain FFM02 and FFM01/06 in the northwestern part of the tectonic lens (Petersson et al. 2024), and the high percentage of non-flowing open fractures (Follin et al. 2025).

3.1 Hydraulic interferences in the uppermost bedrock

The maps shown in Figure 3-1 and Figure 3-2 present the cross-hole pumping tests run 2018 in percussion boreholes HFM43 and HFM33, respectively (ID 8 and 9 in Table 3-2). Observed hydraulic responses are presented in terms of a "response index", r^2/dt (m^2/s). The ratio is proportional to the hydraulic diffusivity, T/S, i.e., $T/S \cong r^2/dt$ (m^2/s). Thus, the sketched ellipses enclose hydraulic diffusivity values deemed as "Excellent, High or Medium". Detailed borehole investigations reveal that the open fractures yielding such values are subhorizontal, often have distinct apertures of several millimetres, transmissivities of the order of 10^{-4} m^2/s or greater, and occur between 50-150m depth.

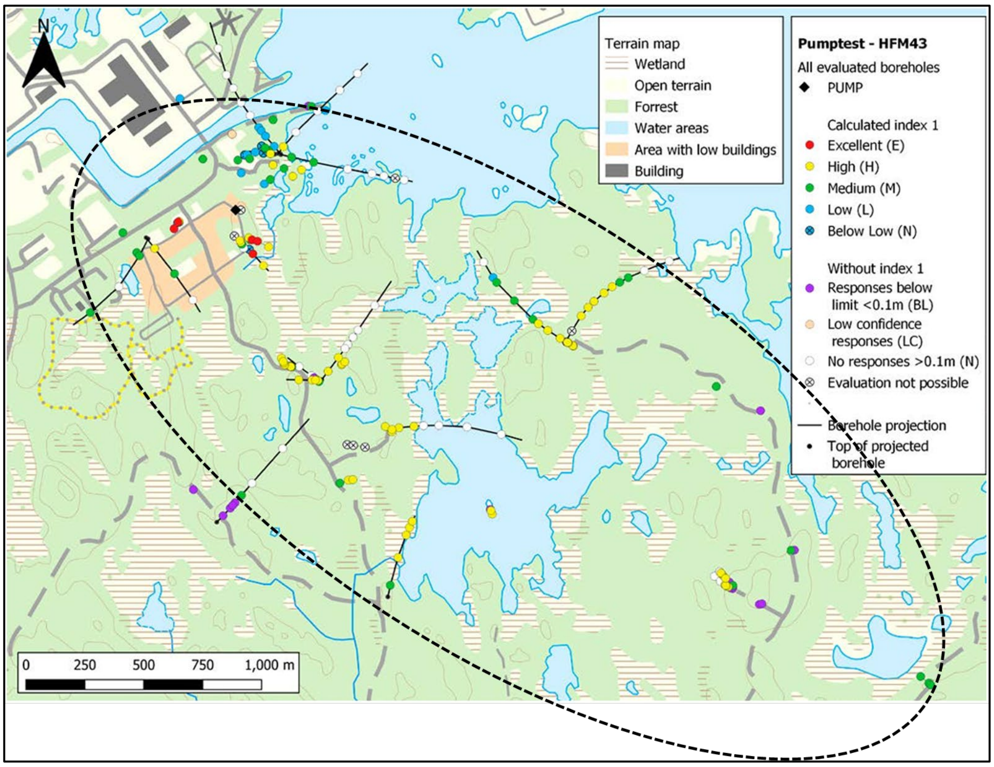

Figure 3-1. *The sketched ellipse includes hydraulic responses classified as "Excellent, High or Medium" during the 2018 cross-hole pumping test in HFM43 (♦). Notably, HFM43 intersects a flowing structure at c. 106m depth with a distinct aperture of 40mm and a transmissivity of 5.3E-4 m^2/s. Modified after Föhlinger et al. (2020).*

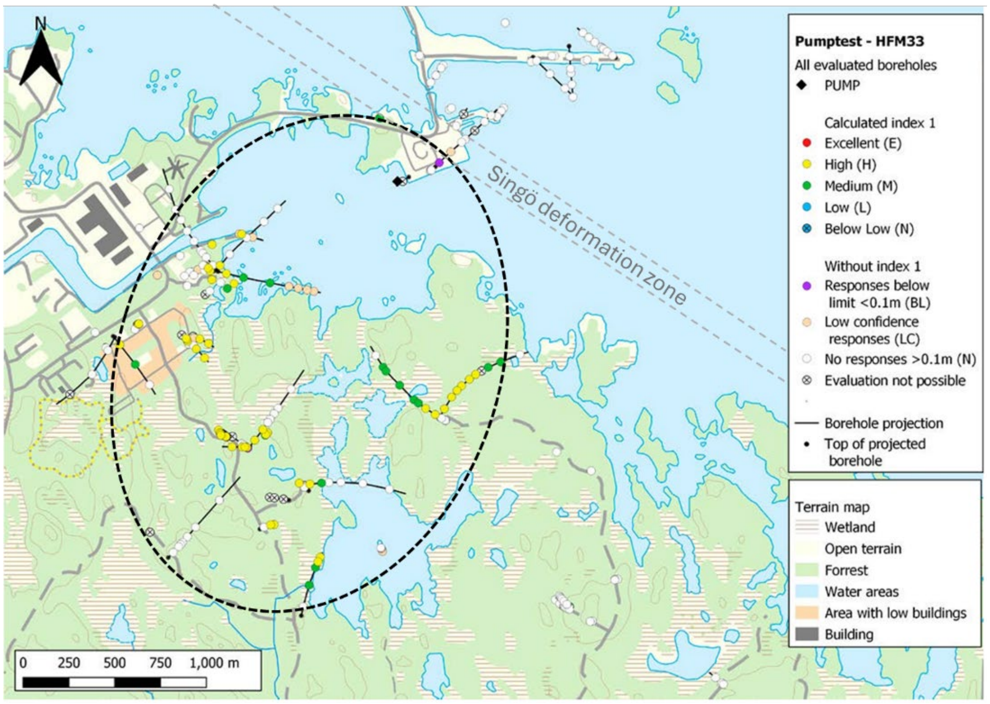

Figure 3-2. *The sketched ellipse includes hydraulic responses classified as "Excellent, High or Medium" during the 2018 cross-hole pumping test in HFM33 (♦). Notably, HFM33 intersects a flowing structure at -136m elevation with a distinct aperture of 8mm and transmissivity of 2.6E-4 m^2/s. Moreover, no hydraulic responses were observed northeast of the Singö deformation zone. Modified after Föhlinger et al. (2020).*

The sketched ellipses in Figure 3-1 and Figure 3-2 support the lateral cross-hole hydraulic responses reported in SDM-Site (ID 5 and ID 6 in Table 3-1), see Figure 3-3. In conclusion, all cross-hole tests listed in Table 3-1 and Table 3-2 reveal a network of well-connected, transmissive, subhorizontal fractures. The network extends throughout fracture domain FFM02, into fracture domain FFM05 all the way up to the Singö deformation zone, where it stops (ID 7 in Table 3-1 and ID 9 in Table 3-2). Tentatively, the network also crosses the gently dipping deformation zone ZFMA2 and further into fracture domain FFM03. Notably, hydraulic responses have also been observed at large depths along the steeply dipping deformation zone ZMFENE0060 and the gently dipping deformation zone ZFMA2 (ID 5 and ID 6 in Table 3-1). The deep responses in mind are shown as squares (☐) in Figure 3-3.

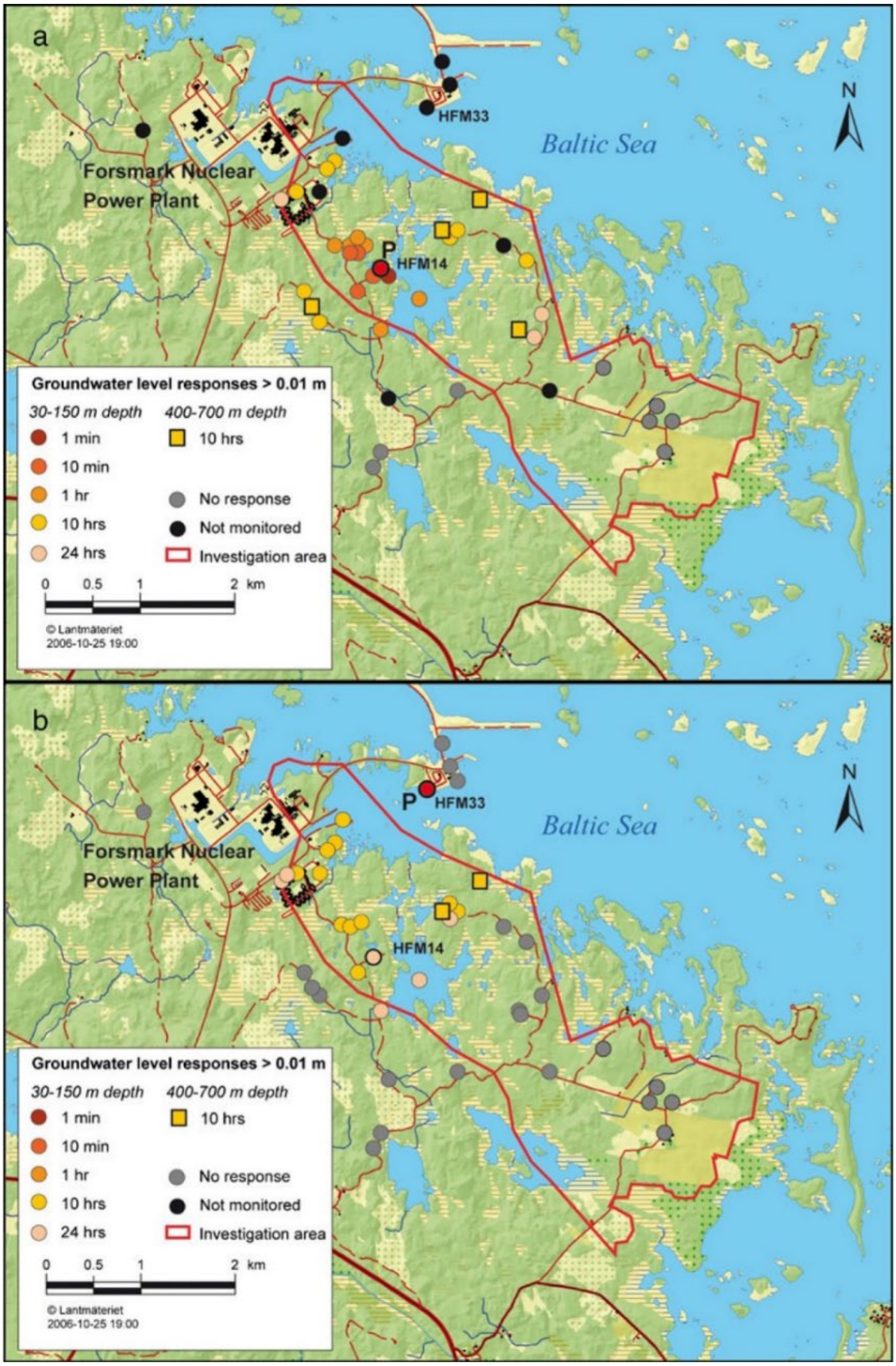

Figure 3-3. *Response times in the crystalline bedrock: a) the three-week long cross-hole hydraulic test conducted in borehole HFM14 (P) in 2006 (ID 5); b) the two-week long cross-hole hydraulic test conducted in borehole HFM33 (P) in 2007 (ID 6). Borehole locations with responses in the uppermost c. 30-150m of rock are shown as circles. Interferences in the interval −400m to −700m elevation are shown as squares. From Follin and Hartley (2014).*

Figure 3-4 shows an oblique view to northeast of fracture domain FFM02. Fourteen cored boreholes have been drilled in this area posterior to SDM-Site (ID10 in Table 3-2). Petersson et al. (2024) suggests a split of FFM02 into two subdomains: FFM02U and FFM02L, where FFM02U lies above FFM02L. FFM02U is c. 20-30m thick. The thickness of FFM02L varies. The thickest part of FFM02L reaches depths below 200m and is overlain by fracture domain FFM03. Fracture domains FFM01/06 (not shown in Figure 3-4a) underlie FFM02U, FFM02L and FFM03. Acquired structural data in boreholes and along the walls of the inlet channel (ID 1 in Table 3-1) reveal that the rock masses associated with FFM02U, FFM02L and the uppermost part of FFM01/06 in the northwestern part of the tectonic lens are sheeted by subhorizontal joints with distinct apertures. Petersson et al. (2024) conclude that the spacing between identified sheet joint traces increases with depth and that near-surface sheet joints, i.e., above 50m depth, are more affected by non-tectonic processes, e.g., glacial processes, than deeper sheet joints, i.e., below 100m depth.

Figure 3-5 shows a tentative 3D structural model of identified sheet joint *traces* in the inlet channel and in the boreholes intersecting the uppermost bedrock in the northwestern part of the tectonic lens (Hartley et al. 2021).

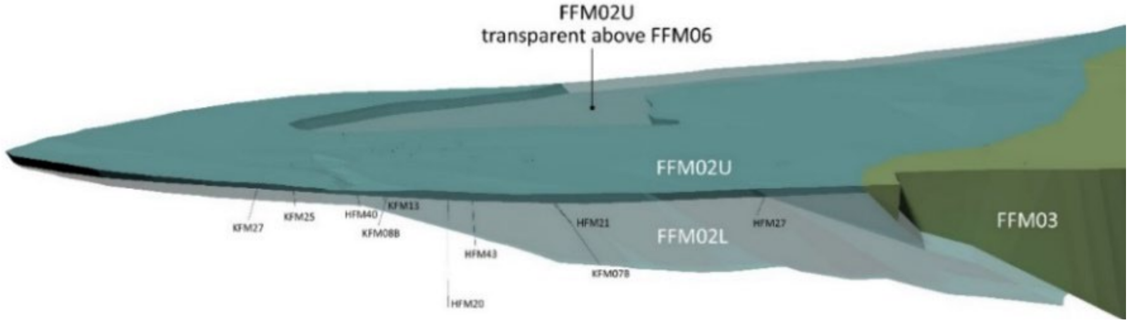

Figure 3-4. *Oblique view to northeast showing the relationship between fracture subdomains FFM02U (upper) and FFM02L (lower). Fracture domain FFM03 is shown for reference (cf. Figure 1-2). FFM02U lies on top of FFM02L, which lies on top of fracture domains FFM01/06. FFM02U is transparent above FFM02L to display the extent of FFM06 below FFM02L. All boreholes used to define the boundary between FFM02U and FFM02L and between FFM02L and FFM01/06 are not visible in this view. From Petersson et al. (2024).*

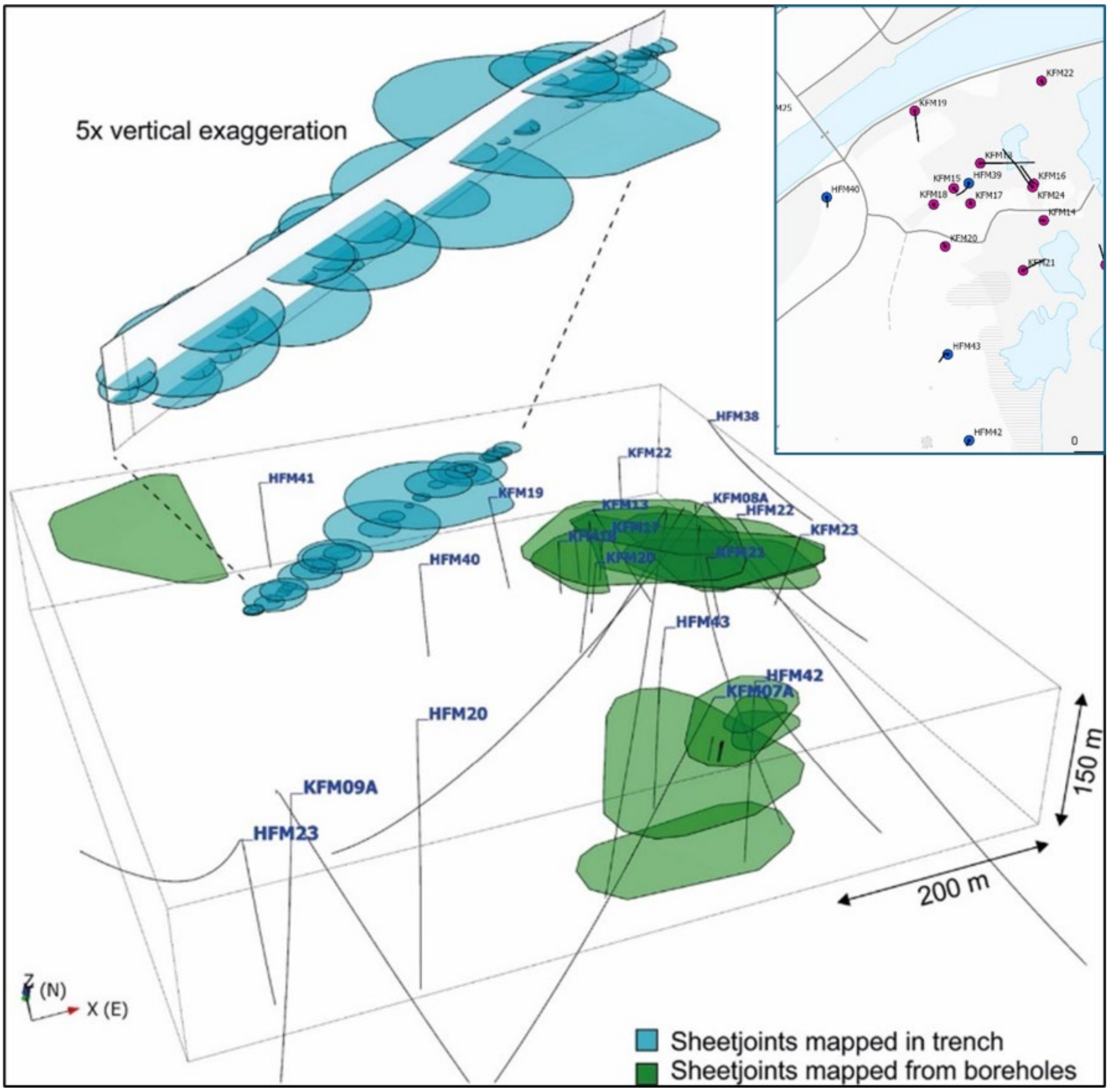

Figure 3-5. *Oblique view of a tentative 3D structural model of identified sheet joint traces described in Petersson et al. (2024). From Hartley et al. (2021).*

3.2 Hydraulic resistance for flow transverse the regional Singö deformation zone

The absence of hydraulic responses transverse the c. 180m thick Singö deformation zone associated with the cross-hole tests listed as ID 7 in Table 3-1 and ID 9 in Table 3-2 are portrayed in Figure 3-2 and Figure 3-3. Though none of these cross-hole tests proves that the Singö deformation is impervious in a direction transverse to its strike, together they strengthen the hypothesis that the structural-hydraulic properties of the tectonic lens may be bounded, at least locally. In other words, future hydrological and hydrogeological modelling must consider three different structural-hydraulic scenarios of the Singö deformation zone to assess its effect on exit locations in particle tracking simulations: 1) pervious in all directions, 2) impervious in all directions, and 3) pervious in all directions in its uppermost part only, e.g., down to -30m elevation, but elsewhere impervious. It is anticipated that these scenarios bracket both the conceptual uncertainties and the parameter uncertainties at hand.

3.3 Linear intensity and transimissivity of open fractures

The linear intensity of open fractures in cored boreholes, $P_{10,o,corr}$ (m^{-1}), is a key quantity in DFN modelling. The fourteen cored boreholes drilled into FFM02U, FFM02L and FFM01/06 reach on average a depth of c. 100 m. Unlike the cored boreholes drilled in SDM-Site, the fourteen boreholes have noticeably short steel casings installed into the bedrock and hence provide important structural-hydraulic information for the uppermost bedrock. This information was not available for SDM-Site, since most boreholes were cased to c. 90 m depth. The solid blue and purple lines in Figure 3-6 depict that the average values of $P_{10,o,corr}$ above 90m depth (equivalent to c. –90 m elevation) in the fourteen cored boreholes are significantly higher than the corresponding values assumed in the absence of real data in SDM-Site, i.e., the dashed green and orange lines.

Figure 3-7 shows evaluated specific capacities (so-called PFL transmissivities) of the flowing open fractures identified in the boreholes investigated with Posiva flow log (PFL) method in terms of cumulative distribution functions (CDFs). Here, 'Steeply dipping' represents all flowing fractures that are not subhorizontal, and the subhorizontal fractures are divided into two categories: 'Sheet joints' and 'Remaining Sub HZ'. Remarkably, only ten percent of the linear intensity of open fractures observed in the boreholes intersecting FFM02U and thirteen percent of those observed in the boreholes intersecting FFM02L are detected as flowing with the PFL method. That is, most of the open fractures, including sheet joints with distinct apertures, identified in the fourteen boreholes penetrating the uppermost bedrock are not continuously flowing implying they have one or several geometrical-hydraulic constraints, e.g., they are unconnected (isolated), have hydraulic chokes (poor geometrical connectivity, fracture infilling etc.), or have transmissivities below the lower measurement limit of the PFL tool.

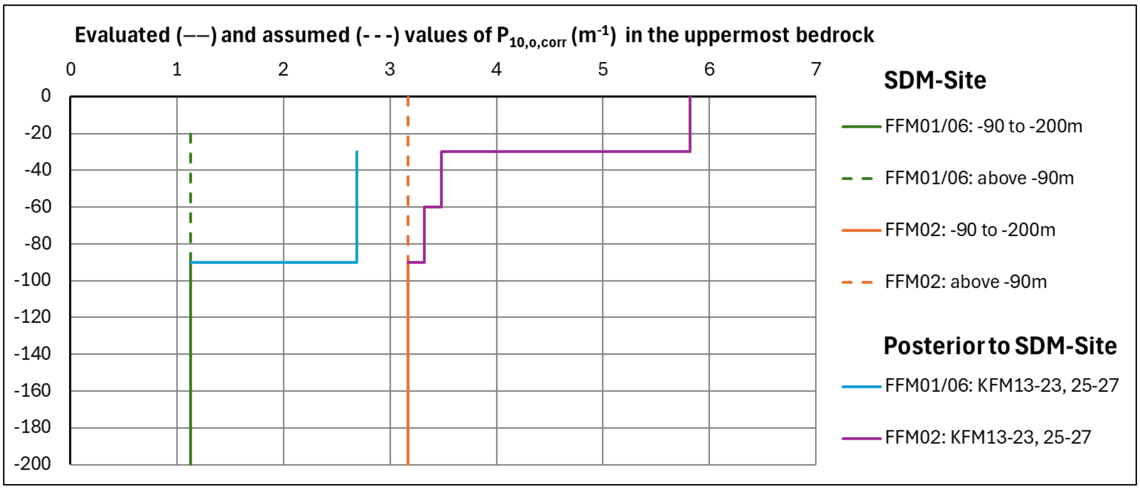

Figure 3-6. *Linear intensity of open fractures in cored boreholes, P10,o,corr (m–1), above –90 m elevation in FFM01/06 and FFM02, respectively. The solid green and orange lines represent the evaluated average values for FFM01/06 and FFM02 between –90 m and –200 m elevation, respectively, in SDM-Site. The dashed green and orange lines represent the corresponding assumed values in SDM-Site above –90 m elevation. The solid blue and purple lines represent the evaluated average values of P10,o,corr above –90 m elevation in the fourteen cored boreholes. From Follin et al. (2025).*

FFM02U

FFM02L

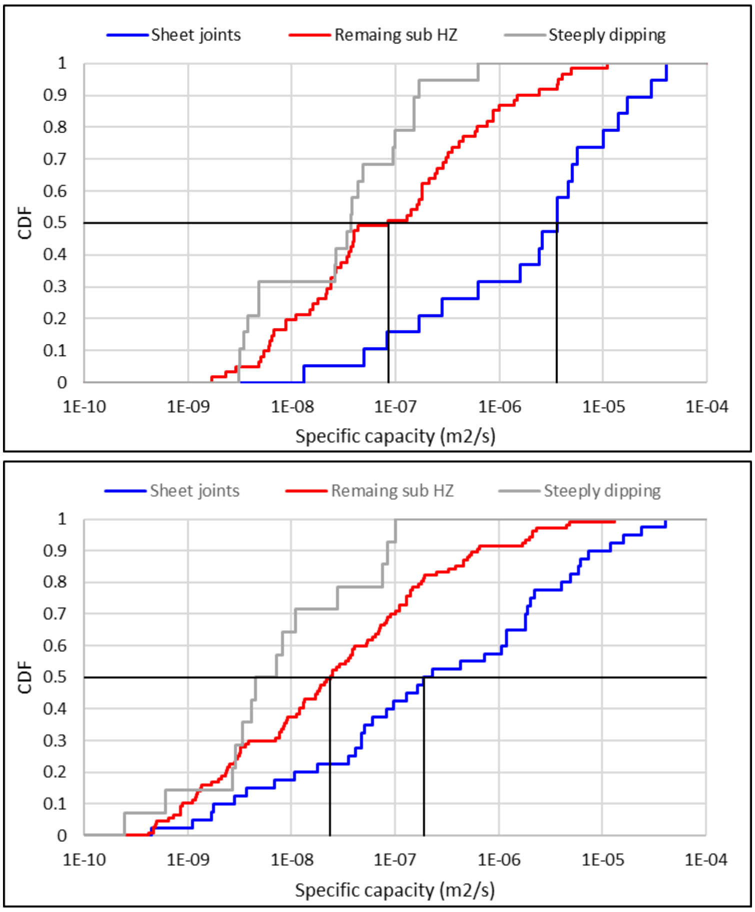

__Figure 3-7.__ Cumulative distribution functions of the specific capacity, Q/Δh, for open connected fractures detected with the Posiva Flow Log in eleven boreholes. 'Steeply dipping' represents flowing fractures that are not subhorizontal. The flowing subhorizontal fractures are divided into two categories: 'Sheet joint' and 'Remaining Sub HZ'. From Follin et al. (2025).

To conclude, the significant lateral hydraulic responses observed in the large-scale cross-hole pumping tests presented above are not limited to fracture domains FFM02U and FFM02L. Data reveal that cross-hole hydraulic responses are also observed in fracture domains FFM01, FFM06 and FFM05. Tentatively, responses are also observed across the hydraulically important, gently dipping deformation zone ZFMA2, and further into fracture domain FFM03. However, no responses have been observed across the thick Singö deformation zone (yet). Notably, the hydraulic responses observed in the large-scale cross-hole pumping tests have been acquired in open boreholes, or in boreholes with one or more packers. The observation boreholes are on average c. 150m deep. Evidently, the hydraulic responses observed in the large-scale cross-hole pumping tests are not prohibited by strong local hydraulic heterogeneities as observed in the uppermost c. 100m of the bedrock amongst the open fractures, including sheet joints with distinct apertures, identified in boreholes (KFM13-23, 25-27). All in all, this suggests that the hydraulic responses observed in the large-scale cross-hole pumping tests are linked to discrete networks of large, hydraulically heterogeneous, subhorizontal sheet joints. At locations where the subhorizontal sheet joints are ending, or are hydraulically choked, the large-scale connectivity between the subhorizontal sheet joints is possibly upheld by intersections with other, more frequent but shorter and less transmissive, flowing open fractures, e.g., 'Steeply dipping' and 'Remaining horizontal' open fractures.

4 Modelling protocol

4.1 DFN versus ECPM

The proposed protocol for hydrological and hydrogeological flow modelling strives for consistency between the groundwater flow modelling tools used for the Surface (regolith) and Bedrock systems, respectively, regarding relevant performance measures (cf. Section 1.3). To enable comparisons between the different flow modelling tools, the protocol combines different flow modelling concepts: porous (continuous) medium concepts and discrete (discontinuous) medium concepts. It is noted that current computational limits of using complex discrete fracture network (DFN) models for flow and transport modelling often make equivalent continuous porous medium (ECPM) models the only practical approach for integrated hydrological and hydrogeological flow modelling. Notably, the protocol suggests that the hydraulic interaction between the regolith (the porous medium) and the bedrock (the discrete medium) is managed through 'upscaling' – a form of averaging in which DFN model realisations are transformed into ECPM model realizations (Figure 3-1). The upscaling techniques considered in this report are based on the comparisons in Hartley et al. (2021) and described in Section 4.3.

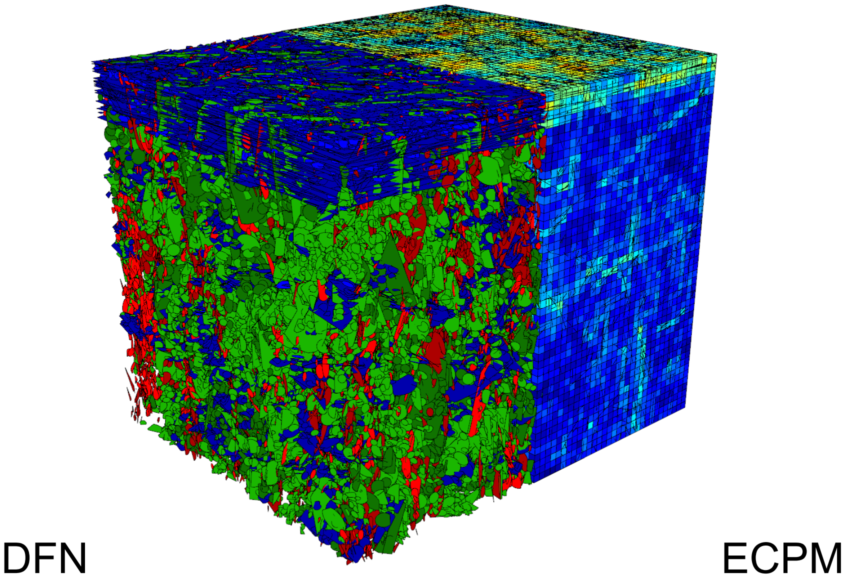

Figure 4-1. *Oblique view of an example computer-made illustration showing the concept of upscaling, a form of averaging in which a discrete fracture network (DFN) model (left side) is transformed into an equivalent continuous porous medium (ECPM) grid model (right side). In this figure, the depicted fractures are simply coloured by orientation – blue represent subhorizontal fractures and red and green represent steeply dipping fractures in two different mean directions. The high frequency of subhorizontal fractures near the upper boundary represent sheet joints. The grid cell colours reflect an upscaled continuum property – in this example the spatial variation in colours reflect the amount of fracture surface area within each grid cell, where red represents "maximum intensity" and dark blue represents "minimum intensity". Grid cells' continuum properties of importance for groundwater flow are, e.g., kinematic porosity and hydraulic conductivity. From Simon Libby (pers. comm. 2023).*

4.2 Workflow

The proposed protocol for integrated hydrological and hydrogeological flow modelling is shown in Figure 4-2. The workflow is divided into two stages, A and B. The flow modelling in Stage A is made with discrete media concepts and modelling tools and in Stage B with porous media concepts and modelling tools.

The generation of fractures in Stage A requires a conceptual framework for fractures of different types and scales, e.g., one of the two DFN concepts briefly described in Section 2.3.2 – DFN-2008 and DFN-2020 (Selroos et al. 2022). However, the workflow of the protocol is principally independent of the DFN concepts used, provided that the generated stochastic DFN model realisations are structurally conditioned and hydraulically (or hydromechanically) calibrated prior to ECPM upscaling.

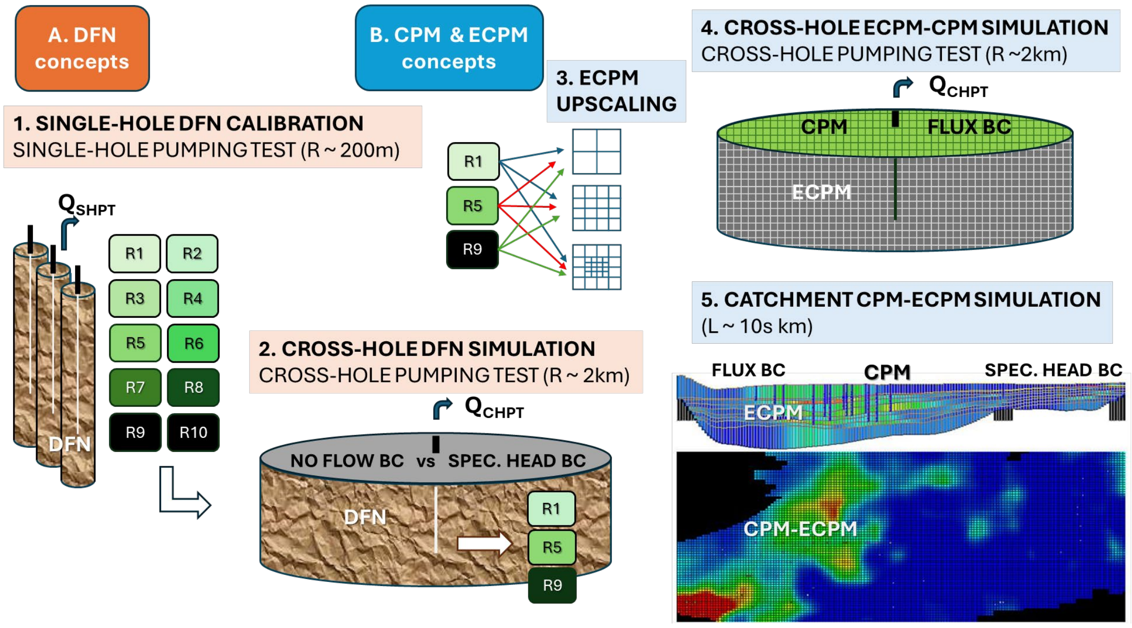

__Figure 4-2.__ Illustration of the proposed protocol for integrated hydrological and hydrogeological flow modelling. The workflow is divided into two stages, A and B. The flow modelling in Stage A is made with discrete media modelling concepts and tools and in Stage B with porous media modelling concepts and tools. The reasons for using different top boundary conditions in Stages A and B are explained in the text.

A. Multiple (in the example below we use ten) catchment-scale DFN model realisations are generated using a fracture generator, e.g., FracMan® (https://www.wsp.com/en-US/services/fracman). Each DFN model realisation is a conditioned, i.e., semi-stochastic, representation of the geometrical properties of observed fracture traces on outcrops and/or in boreholes.

   1. First, several single-hole pumping tests (Q_{SHPT}) are simulated for each DFN model realisation. Cylindrical "cut-out" models with a radius of 200–250m are created around each borehole and steady-state constant-density flows are simulated using a flow solver, e.g., PFLOTRAN (https://pflotran.org). The boundary conditions are a zero head on the lateral surface, a specified drawdown (Δh) in the pumped borehole, e.g., 10m, and no-flow conditions on the top and bottom faces. The inflow at each fracture intersection with the borehole as well as the total inflow (discharge) are calculated. For ***N*** single-hole tests (boreholes), this step yields ***N*** times ten flow simulations per model iteration. The ensemble of flows over the (***N***×10) simulations are collated by fracture domain, or borehole, and compared with corresponding metrics of the authentic single-hole pumping tests. The DFN model parameters are adjusted, and the flow simulations are iterated until a match is achieved in a statistical sense, e.g., a match of the median value over the ensemble of realisations. For DFN-2008, the key parameters to adjust are those of the fracture size distribution and the transmissivity parameterisation. For DFN-2020, several parameters are adjusted including fracture openness and the chosen model for hydromechanical coupling. Figure 4-3 illustrates the workflow.

2. Second, at least one of the cross-hole pumping tests conducted within the local model domain in Forsmark is simulated. The most significant tests, as listed in Tables 3-1 and 3-2, are ID 5, ID 6, and ID 8. For each selected cross-hole pumping test borehole, a cylindrical “cut-out” model domain with a radius of at least 2,000 m is created. Steady-state, constant-density flow is then simulated within each domain. The resulting drawdowns (Δh) in nearby observation boreholes are compared with corresponding values at shut-in from the actual cross-hole pumping tests.

   Realistic boundary conditions must be assigned to the sides of the cylindrical model domain. In general, all types of boundary conditions strongly influence the calculated interferences, particularly the condition applied to the top face. However, at this stage of the protocol, there is no integration with the Surface system yet. To assess the implication of this constraint, two simplified boundary conditions are considered, as illustrated in Figure 4-2: **no-flow** and **specified head**. A no-flow boundary condition represents confined conditions with no vertical leakage, typically resulting in greater lateral interferences. In contrast, a specified head boundary condition can serve as a proxy for simulating leakage (or "recharge") from the Surface system into the Bedrock system (cf. Figure 1-3). When a no-flow condition is applied to the top face, the boundary conditions at the lateral and bottom surfaces of the domain become more influential than when a specified head is used. Step 2 is repeated for each cross-hole pumping test, each DFN model realization, and each boundary condition combination.

   Although the DFN model realizations analysed in Stage A.1 are geometrically conditioned and flow calibrated in a statistical sense, i.e., they are statistically equalprobable, it is noted that this calibration is not necessarily valid beyond the extent of the cylindrical “cut-out” models with a radius of 200–250 m used in that stage. In other words, all of the equalprobable DFN model realisations in Stage A.1 may not be considered equally reasonable in the comparison with DFN cross-hole pumping test data, which uses a cylindrical “cut-out” model domain with a radius of at least 2,000 m. Ideally, all of the equalprobable DFN model realisations in Stage A.1 are approved also in Stage A.2 and hence propagated to Stage B, Step 3. If the number of approved DFN model realisations is large, it may be reasonable to start with an excerpt, e.g., R1, R5, and R9 in the depicted example.

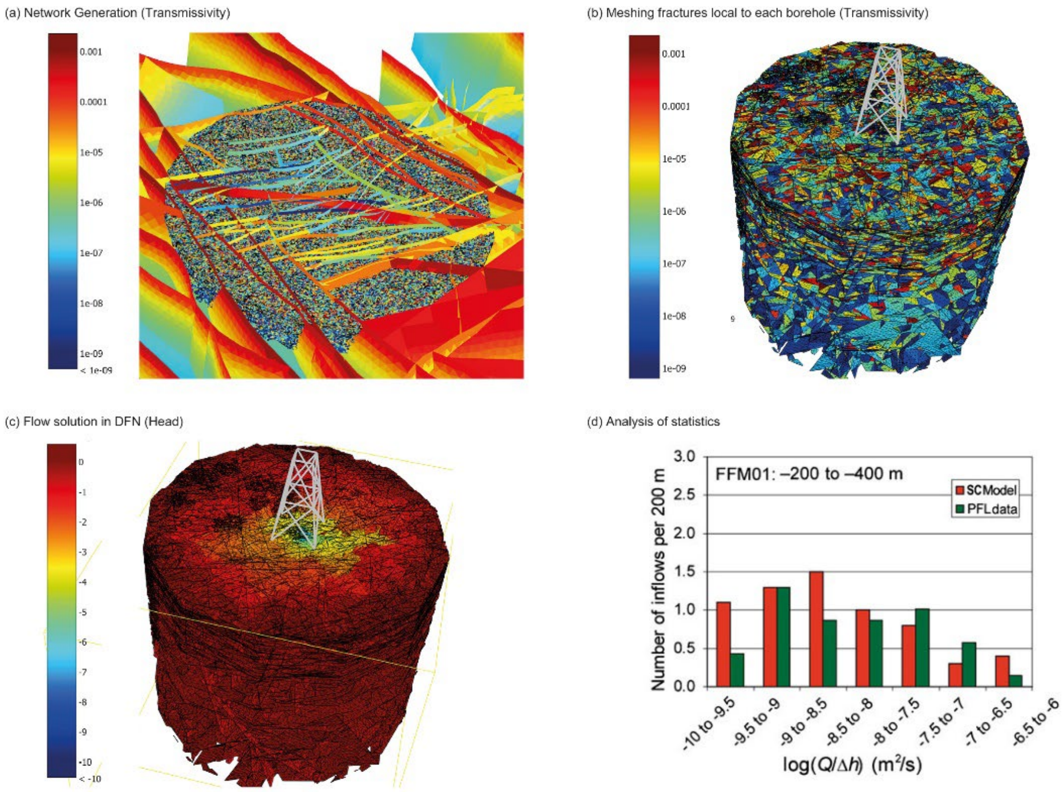

Figure 4-3. *Principal workflow of single-hole pumping test simulations: a) generation of a DFN model realisation inside the local model domain (cf. Figure 1-2); b) gridding of borehole-scale model; c) single-hole inflow simulation; and d) calibration. Modified after Follin et al. (2007b) and Hartley et al. (2021).*

B. Stage B consists of three steps: Upscaling, cross-hole pumping test simulations, and catchment-scale flow simulations. Historically, SKB has used two modelling tools in parallel for porous medium flow simulations: DarcyTools (Svensson et al. 2010) and MIKE SHE (DHI 2023). This parallel approach reflects the distinct capabilities of each tool. DarcyTools is developed for simulating groundwater flow and solute transport in bedrock, while MIKE SHE is designed for simulating a broader range of hydrological processes, including precipitation, evapotranspiration, groundwater flow in the regolith, and groundwater-surface water interactions. DarcyTools is a finite volume-based code capable of handling both structured and unstructured grids, providing flexibility for complex geological settings. MIKE SHE uses a classic finite difference approach, restricting it to structured grids. (At the time of writing this report, no final decision has been made regarding the continued use of MIKE SHE in future projects.)

3. The propagated DFN model realisations from Stage A.2 are upscaled to ECPM grid model realisations intended for DarcyTools and MIKE SHE, respectively. Before upscaling, all isolated fractures including isolated clusters of fracture are removed. In other words, each DFN model realisation is upscaled to two tool-dependent ECPM grid model realisations, one intended for DarcyTools, and another intended for MIKE SHE. It is noted that different upscaling methods and grid resolutions are used with DarcyTools and MIKE SHE. Section 4.3 revisits the upscaling methods assessed in Hartley et al. (2021).

4. The cross-hole pumping tests simulated with PFLOTRAN in Stage A.2 are repeated with both DarcyTools and MIKE SHE for each ECPM grid model realisation of the Bedrock system derived in Stage B.3. Notably, the boundary conditions used in Stage A.2 are unchanged in Step B.4. If unrealistic flow solutions are obtained with all ECPM grid model realizations compared with the DFN model realisations in Stage A.2, this might be an indicator of insufficient (i.e., too coarse) ECPM grid model resolutions. To investigate if this is the reason, the upscaling in Stage B.3 could be repeated using finer grid resolutions. An often-used rule of thumb in upscaling is that the size (Δ in m) of the smallest ECPM grid cell should be of the same order, or less, than the diameter of the shortest connected open fractures ('cof') DFN, i.e., $\Delta \leq 2\, r_{min,cof}$.

5. In Stage B.5, the deterministic CPM ('continuous porous media') model for the Surface system presented in Section 2.5.2 is merged with each ECPM grid model realisation developed for DarcyTools and MIKE SHE, respectively, in Stage B.4. The cross-hole pumping tests simulated with PFLOTRAN in Stage A.2 are repeated using DarcyTools and MIKE SHE in parallel, however with a flux-type top boundary condition to increase the realism. Atmospheric, surface and near-surface processes are modelled on a diurnal basis in the flow modelling with MIKE SHE. A transient Cauchy (mixed) boundary condition might be a reasonable proxy with DarcyTools. Tentatively, pseudo steady state flow (mimicking a long-time flux average over several years) might be used in DarcyTools as the effects of diurnal changes in surface and near-surface processes typically decrease with depth (Section 2.6).

   If the flow solutions obtained in Stage B.5 with DarcyTools and MIKE SHE differs significantly, the reason(s) must be investigated and resolved before proceeding to Stage B.6.

   Figure 4-4 and Figure 4-5 show examples of the modelling and calibration activities included in Step 4. Figure 4-4 illustrates an octree DarcyTools grid intended for modelling the cross-hole pumping test conducted 2018 in borehole HFM43 (ID 8 in Table 3-2). Figure 4-5 compares predicted and measured changes in groundwater levels in available monitoring boreholes in the bedrock at the shut-in of the cross-hole test conducted in 2006 in borehole HFM14 (ID 5 in Table 3-1). Notably, the parameterisation of the CPM model for the Surface system in Figure 4-5 is the same for all ECPM grid model realisations.

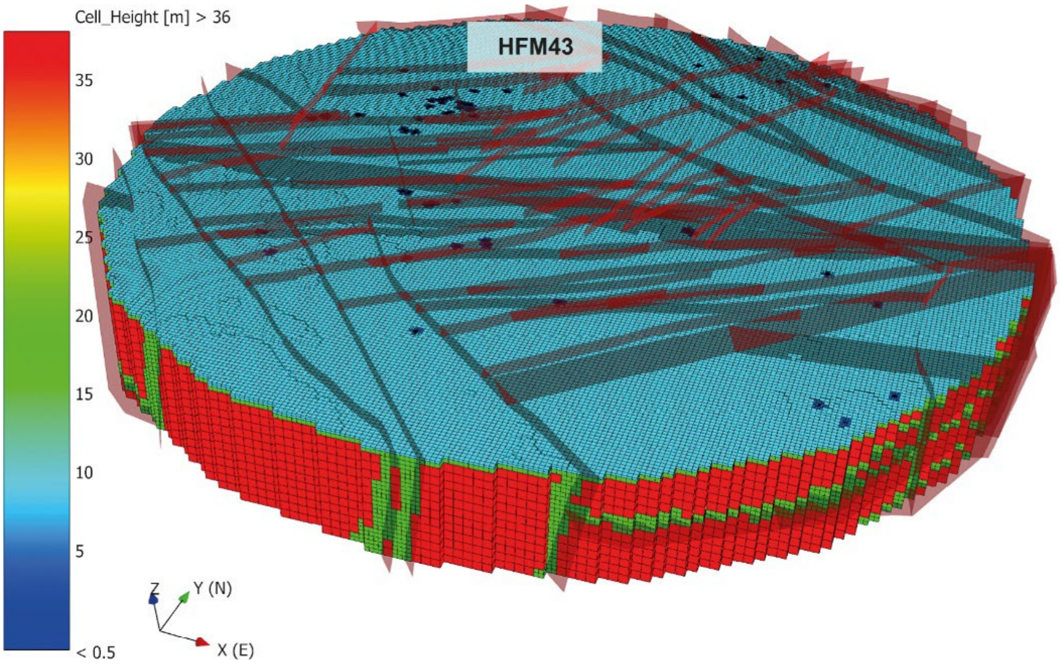

***Figure 4-4.** Oblique view of an octree DarcyTools grid intended for modelling the three-week long cross-hole pumping test in percussion borehole HFM43 (ID 8 in Table 3-2). The regolith is shown in blue, deterministically modelled deformation zones and sheet joints in green, and the rock mass outside deformations zones (fracture domains) in red. The grid is 3,800 m in diameter and up to 465 m thick. Modified after Hartley et al. (2021).*

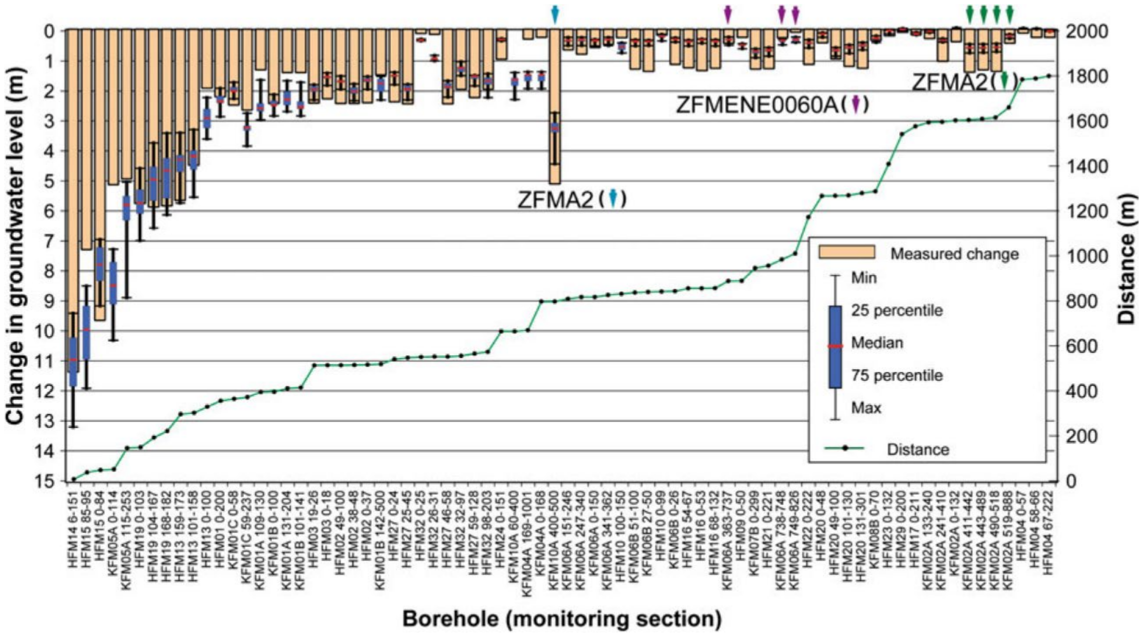

Figure 4-5. *Plot comparing predicted and measured changes in groundwater levels for the 3-week-long cross-hole test conducted in 2006 in borehole HFM14 (ID 5 in Table 3-1). The brown bars represent the measured changes in groundwater levels after 21 days of pumping in HFM 14. The statistics of the simulated changes in groundwater levels taken over ten realisations of the deformation zone model and of the hydrogeological DFN model are shown with blue box-and-whisker plots. From Follin and Hartley (2014).*

6. The flow modelling in Stage B.6 deals with the parameterisation of the deterministic CPM model for the Surface system in DarcyTools and MIKE SHE, and with consistency checks of the calibrated flow models developed in parallel with DarcyTools and MIKE SHE. Stage B.6 has two primary objectives:
   - Assess whether the parameterisation of the deterministic CPM model for the Surface system (Section 2.5.2) implemented in DarcyTools and MIKE SHE remains consistent across the stochastic ECPM grid model realisations for the Bedrock system, using available time series of monitored meteorological and hydrological state variables. Figure 4-6 illustrates the hydrological processes modelled with MIKE SHE and an example of a calculated water balance for the Forsmark site in SDM-Site. Figure 4-7 and Figure 4-8 show two examples of calibration with MIKE SHE in SDM-Site against measured state variables on a diurnal basis – groundwater levels in a regolith borehole and discharge in a brook.
   - Evaluate whether the proposed modelling protocol for integrated hydrological-hydrogeological flow modelling ensures consistency between the concepts and tools used for groundwater modelling in the bedrock and regolith, respectively, see Figure 4-9 through Figure 4-11.

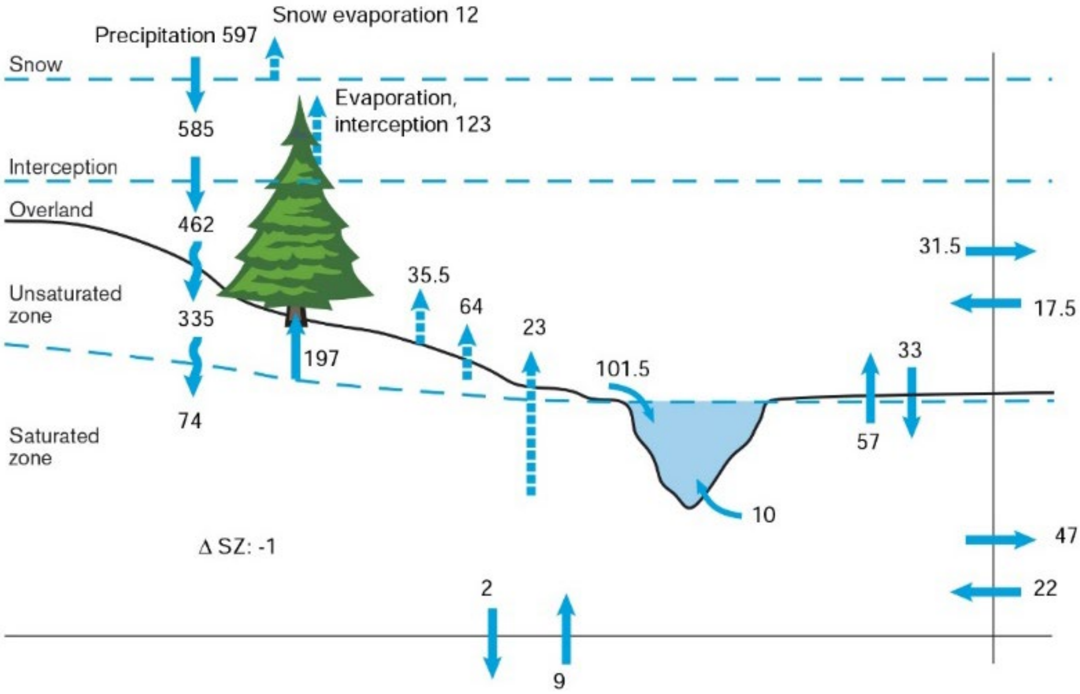

Figure 4-6. *Hydrological processes considered in MIKE SHE with an example of calculated mean annual water balance in mm for a three-year long period in Forsmark. The horizontal arrows crossing the vertical boundary indicate the calculated exchanges of overland flow and groundwater flow across the coastline. From Bosson and Berglund (2006).*

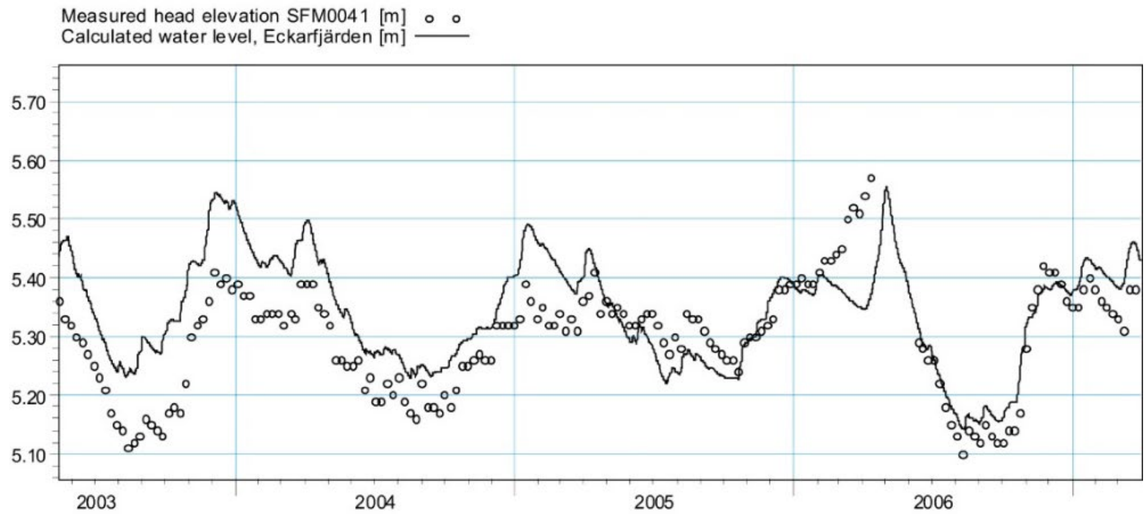

Figure 4-7. *An example of measured groundwater levels in a regolith borehole (o) in relation to calculated groundwater levels (—) for a four-year long period between March 2003 to March 2007. From Bosson et al. (2008).*

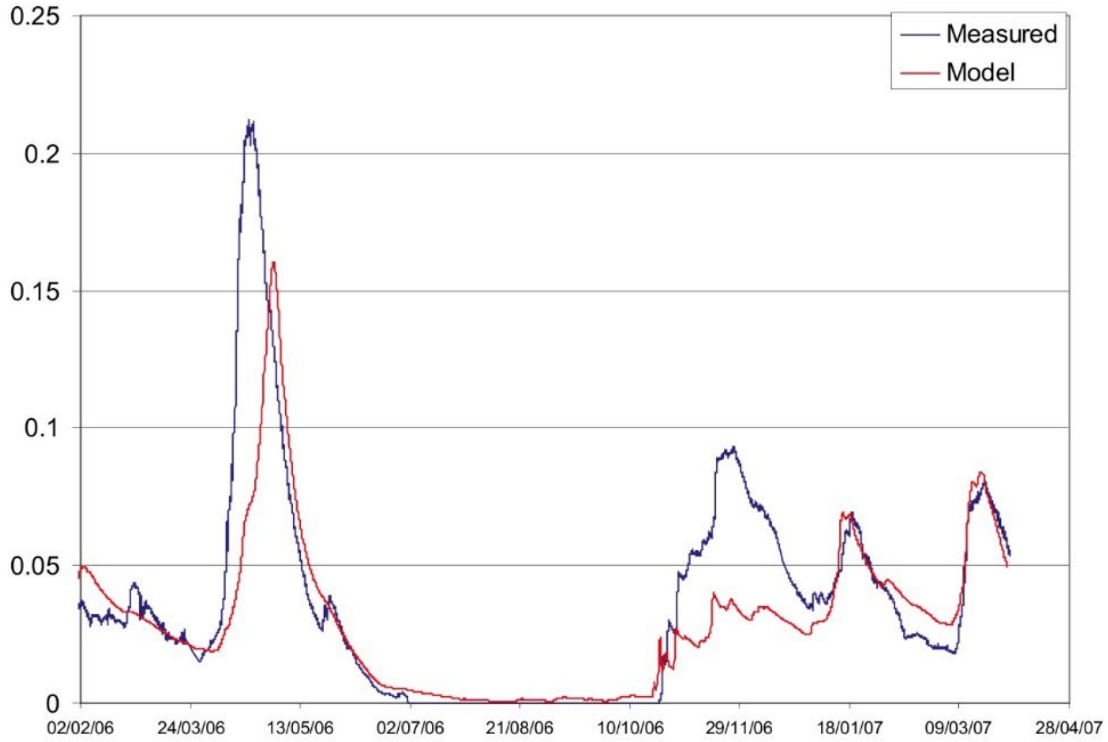

Figure 4-8. *An example of measured diurnal discharge in a brook (—) in relation to calculated diurnal discharge (—) for a one-year long period (2006). From Bosson et al. (2008).*

If the calibration of the CPM model for the Surface system is found to be inconsistent across the ECPM grid model realisations for the Bedrock system, it might be useful to revisit the data underpinning the conceptual model shown in Figure 1-3, including the setup of the associated numerical models in DarcyTools and MIKE SHE. This review should assess whether there are any significant conceptual reasons for the observed inconsistencies. Notably, large, stochastic DFN structures located outside the kilometre-scale model domains modelled in Stages A.2, B.4 and B.5 cannot directly influence these flow simulations in those stages but may impact the catchment-scale flow simulations in Stage B.6.

The second objective can be tested numerically, for example, by examining the extent to which one model can replicate the results of another. Three "prediction and outcome" exercises are proposed using MIKE SHE and DarcyTools in parallel, see Figure 4-9 through Figure 4-11:

- The spatial distribution of groundwater inflow (recharge) and outflow (discharge) areas, for example, across the bedrock-regolith interface (Figure 4-9).
- The magnitudes of groundwater fluxes between ground surface and repository depth (Figure 4-10).
- Particle exit locations (Figure 4-11).

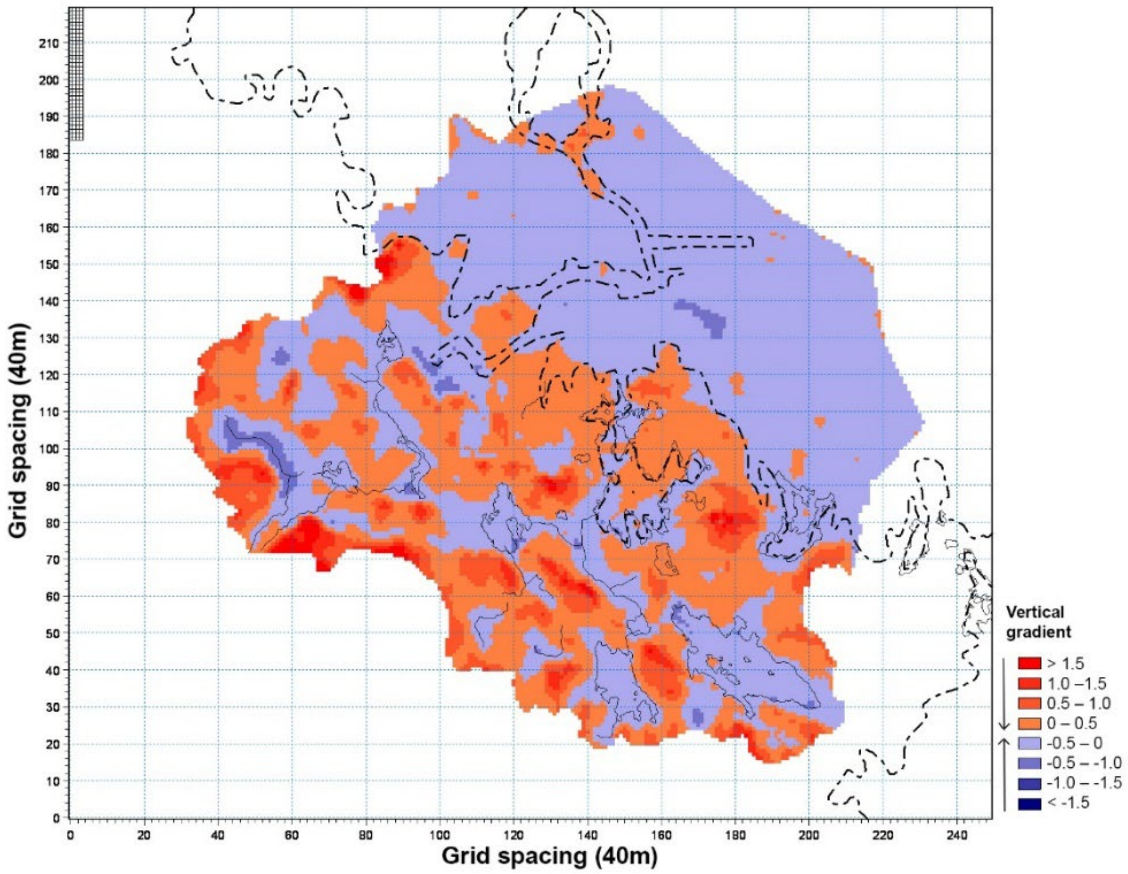

Figure 4-9. *Spatial distribution of the head difference between adjacent grid cells across a horizontal slice at c. −30 m elevation. Downward flow areas (recharge) in red and upward flow areas (discharge) in purple. Modified after Bosson et al. (2008).*

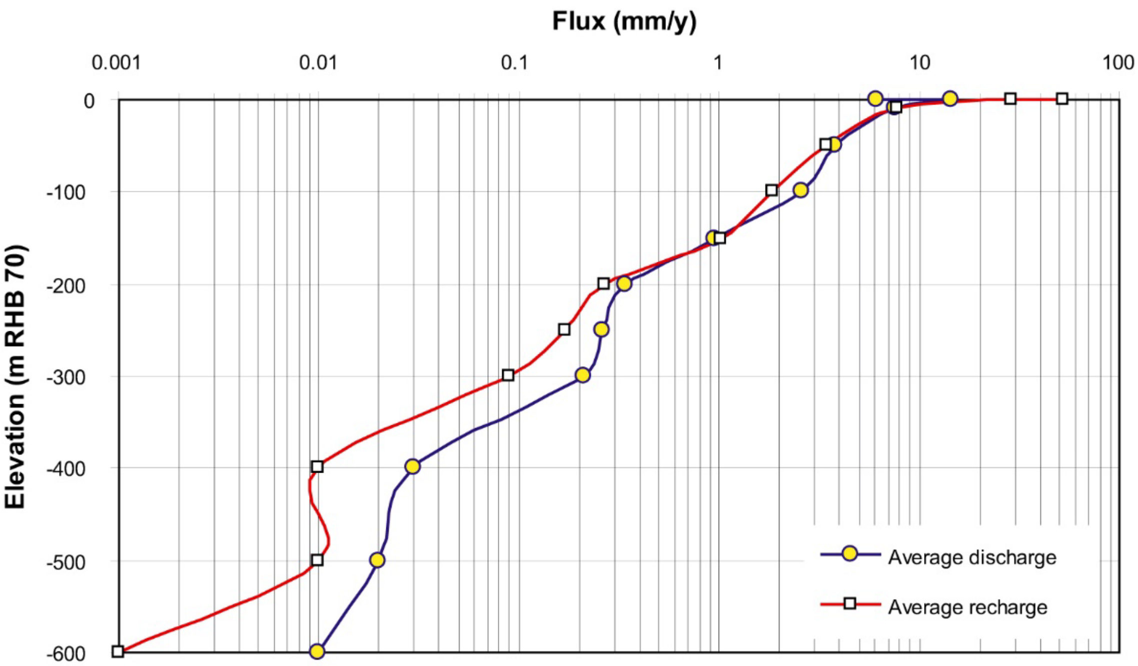

Figure 4-10. *Average values of predicted downward and upward vertical fluxes across a predefined horizontal surface area located at different depths below ground surface. From Follin et al. 2007b).*

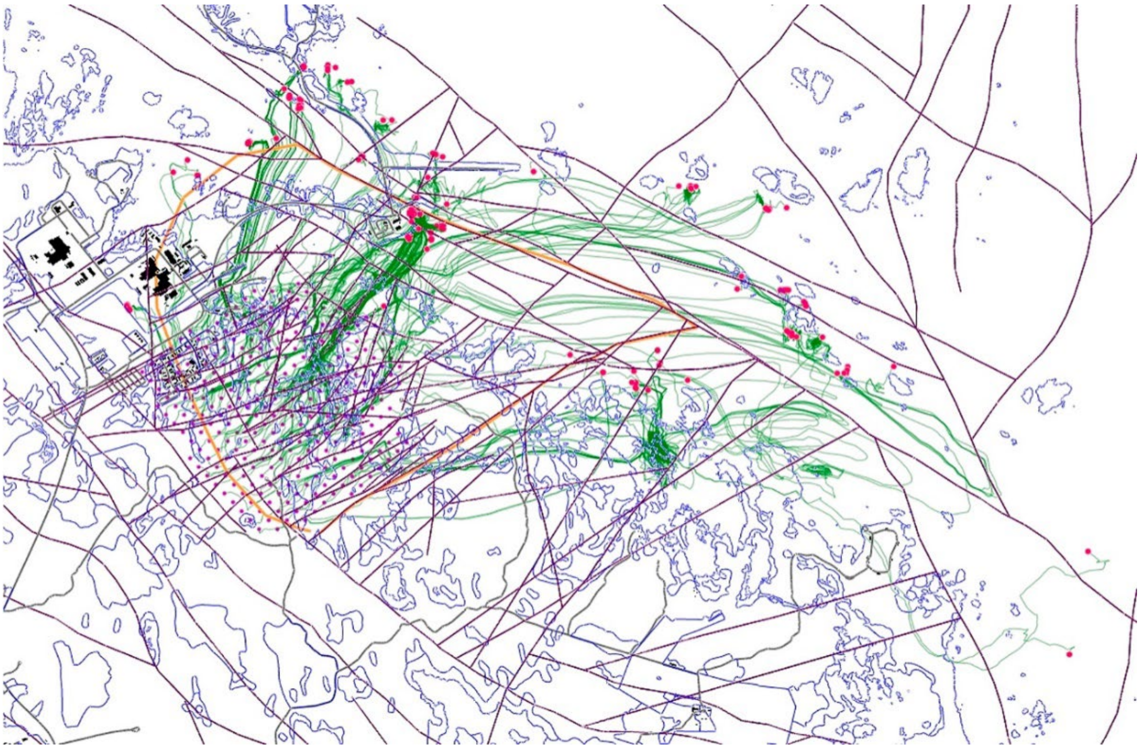

Figure 4-11. *Predicted flow paths (green trajectories) and exit locations at ground surface (red dots) of c. 300 particles released at 500m vertical depth in a 100m by 100m mesh (purple dots). From Follin et al. (2007b).*

4.3 Upscaling

4.3.1 General

ECPM grid models represent an alternative modelling approach that can be computationally less costly as multiple discrete fractures can be represented by a single ECPM grid cell, however, this can easily overestimate flow and smear sub-cell-scale aspects of the DFN, such as directional connectivity and channelling. The current limits of computational power mean that for local- and regional-scale models, ECPM grid models are often the only practical solution/approach. Accurate upscaling methods that produce heterogeneous and anisotropic cell-based permeabilities, as well as porosities and fracture surface area per unit volume, can produce a reasonable approximation of bulk flow and (but to a lesser extent) reasonable solute transport properties. Accurate upscaling methods must capture the geometric connectivity and orientations of fractures, as well as their hydraulic choking (Jackson et al. 2000; Ahmed Elfeel and Geiger 2012; Lei et al. 2015; Chen et al. 2018).

4.3.2 Upscaling methods

Two upscaling methods are implemented in FracMan: The geometric Oda method (Oda 1985, 1986) and a flow-based method (Jackson et al. 2000; Zou et al. 2017), known as 'Block_k' (or 'Cell-k'). Two geometric upscaling method are implemented in DarcyTools, known as GEHYCO Vol method and GEHYCO Area method (Svensson et al. 2010). Upscaling is not implemented in MIKE SHE, but ECPM grid properties calculated with Oda in FracMan can be imported into MIKE SHE. ECPM grid properties calculated with Oda in FracMan can also be imported into DarcyTools.

Both the Oda method implemented in FracMan and the GEHYCO method in DarcyTools are analytical (geometric) methods using only fracture geometry and properties. Flow-based upscaling methods simulate flows across each grid block (cell) and each axial direction, see, e.g., Lei et al. (2015) for a review of methods. Flow-based upscaling methods are intrinsically more accurate, but computationally more intensive.

4.3.3 Comparison of permeabilities calculated with geometric (Oda) versus flow-based upscaling

Hartley et al. (2021) compare permeabilities calculated with geometric (Oda) versus flow-based upscaling for a DFN model realisation with a power-law size distribution and significant inter-fracture heterogeneity, see Figure 4-12. The cubic model domain is split into an array of 10×10×10 array of grid blocks (cells) and both methods are used to upscale each block (cell) to a permeability tensor (k in m^2), as compared in Figure 4-13. Before upscaling, all fractures not connected to the external boundary are removed because the Oda method cannot factor connectivity which is intrinsic for flow-based upscaling.

There is a clear correlation between the two sets of results, but the permeabilities are lower for the flow-based upscaling because the Oda method cannot factor hydraulic choking, which is intrinsic for flow-based upscaling. Values calculated with the Oda upscaling method should therefore be regarded as an upper bound for the true equivalent permeability (or hydraulic conductivity) tensor.

Figure 4-14 shows a cross-plot of the flow-based and Oda-based permeabilities in the x axis direction across all 1,000 blocks (cells). This cross-plot demonstrates that the Oda results are indeed an upper bound for the flow-based results and that most of the cloud values lies within a factor 1–1/3 of the Oda values. The median ratio is about 0.35 and about 70 % of flow-based values are less than half the Oda-based value. This suggests a scaling factor 2-3 between Oda based and flow-based upscaling.

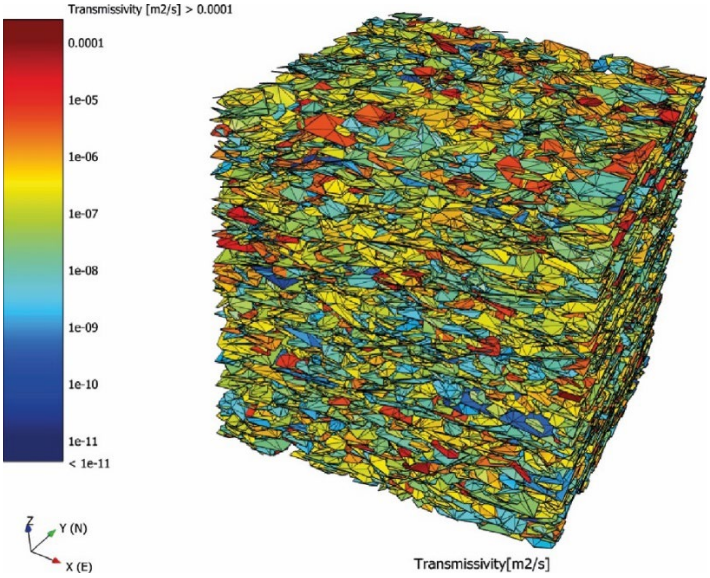

Figure 4-12. *Example visualisation of a DFN model realisation with a power-law size distribution and significant inter-fracture hydraulic heterogeneity inside a cubic model domain. From Hartley et al. (2021).*

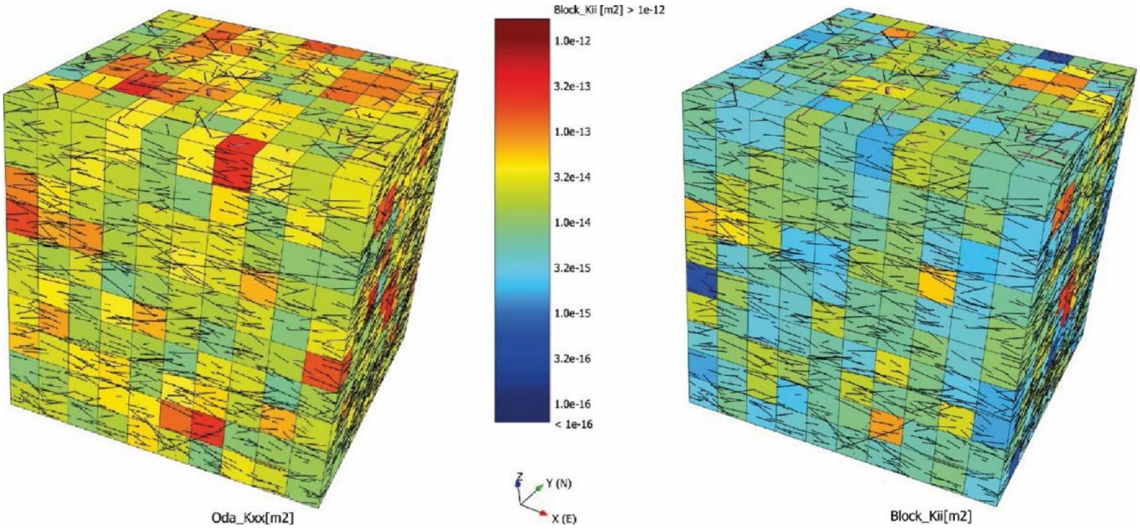

Figure 4-13. *Upscaled* k_{xx} *permeability for a 10×10×10 array of 50-m large grid blocks (cells). (Left) Geometric (Oda) upscaling. (Right) Flow-based upscaling. The permeabilities are lower for the flow-based upscaling because geometric upscaling methods cannot factor hydraulic choking, which is intrinsic for flow-based upscaling. From Hartley et al. (2021).*

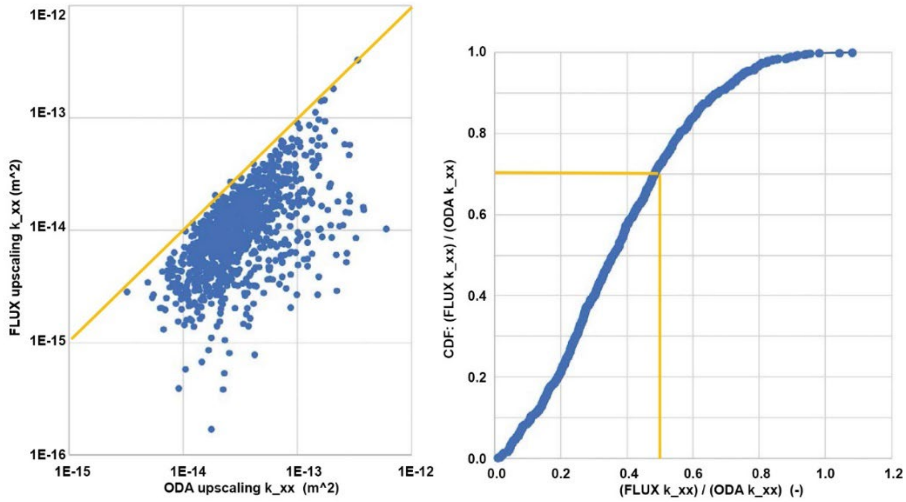

Figure 4-14. *Left: Cross-plot of flow-based versus geometric (Oda) upscaled k_{xx} over all blocks. Right: Cumulative distribution of ratio of flow-based to Oda based k_{xx}. The median ratio is about 0.35 and about 70 % of flow-based values are less than half the Oda-based value. This suggests a scaling factor 2-3 between Oda based and flow-based upscaling. From Hartley et al. (2021).*

4.3.4 Comparison of single-hole pumping test simulations using DFN (FracMan) versus ECPM (DarcyTools)

Hartley et al. (2021) compare simulated values of the total specific capacity ($Q/\Delta h$ in m^2/s) for a single-hole pumping test performed in three DFN model realisations (r1, r2, and r3) using FracMan with three ECPM upscaling methods using DarcyTools:

- An ECPM model with hydraulic conductivity upscaled using the Oda method in FracMan for each DFN realisation (labelled "Oda upscale" in Figure 4-15).
- An ECPM model with hydraulic conductivity upscaled using the GEHYCO Volumetric method for each DFN realisation (labelled "Vol" in Figure 4-15).
- An ECPM model with hydraulic conductivity upscaled using the GEHYCO Area method for each DFN realisation (labelled "Area" in Figure 4-15).

Oda upscaling in FracMan produces a second-order, symmetric, cell-centred hydraulic conductivity tensor. However, due to the way anisotropy is handled in DarcyTools, only the diagonal tensor components (K_{xx}, K_{yy}, and K_{zz}, in m/s) are used. To convert the cell-centred upscaled conductivities for use in DarcyTools, face-centred values are derived using the harmonic mean of the two adjacent cells. This approach accommodates variations in cell size, which is particularly important when using an unstructured octree ECPM grid. In contrast, both the GEHYCO Volumetric and GEHYCO Area upscaling methods import DFN model realisations directly into DarcyTools, with the geometric upscaling performed within the software itself. It should be noted that the GEHYCO Area method is an enhancement of the Volumetric method, designed to reduce the smearing of individual fractures across the cells they intersect and their immediate neighbours.

Figure 4-15 compares simulated values of total specific capacity ($Q/\Delta h$, in m^2/s) for a single hole pumping test, using three DFN model realisations (r1, r2, and r3). The simulations were performed with FracMan (DFN), DarcyTools using FracMan's Oda upscaling, and DarcyTools using the GEHYCO Volumetric and GEHYCO Area upscaling methods.

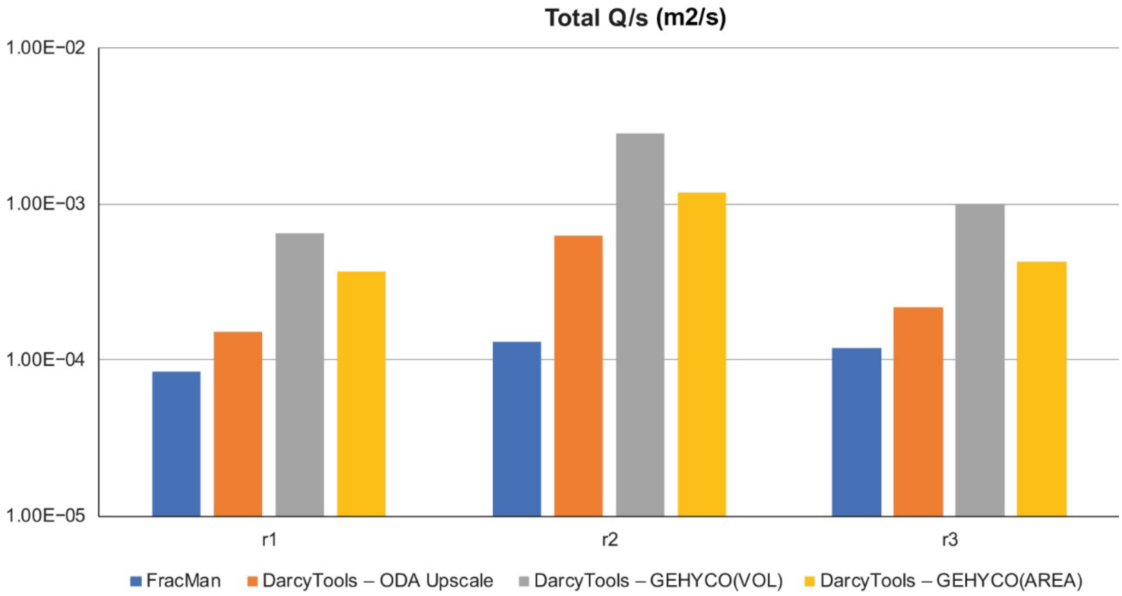

Figure 4-15. *Comparison of simulated values of total specific capacity (Q/Δh, in m²/s) for a single hole pumping test, using three DFN model realisations (r1, r2, and r3). The simulations were performed with FracMan (DFN), DarcyTools using FracMan's Oda upscaling, and DarcyTools using the GEHYCO Volumetric and GEHYCO Area upscaling methods. From Hartley et al. (2021).*

All upscaled ECPM variants produce higher values than the corresponding DFN model simulations, with the Oda upscaling results being the closest. Among the upscaling methods performed within DarcyTools, the GEHYCO Volumetric method yields the highest values—approximately one order of magnitude greater than the DFN results. In contrast, the GEHYCO Area method represents an improvement, with results approximately a factor of two lower than those from the Volumetric approach.

4.3.5 Summary

The choice between using an ECPM or DFN concept for hydrogeological applications in fractured rock is both scale- and problem-dependent. An ECPM approach with relatively coarse spatial resolution (cell size) may be sufficient for studying flow at a regional scale. In contrast, a DFN approach is often preferable when modelling channelised flow through individual fractures. That said, a high-resolution ECPM model can also perform well—sometimes sufficiently so, depending on the specific application.

If an ECPM concept is selected, it is strongly recommended to follow the methodology outlined in this report, with particular attention to the upscaling process. When using the ECPM approach, flow-based upscaling is generally preferred. Alternatively, analytical (geometric) methods such as Oda or GEHYCO can be applied to improve computational efficiency. However, the resulting permeabilities should be rescaled through numerical calibration unless hydraulic choking is explicitly considered.

It is important to note that when using the Oda method, all fractures not connected to the external boundary must be excluded prior to upscaling, as the method does not consider fracture connectivity. In contrast, GEHYCO does account for fracture connectivity.

5 Summary and discussion

The modelling protocol presented in this methodology report strives for consistent performance of the flow modelling tools used for the porous regolith (Surface system) and the fractured bedrock (Bedrock system) inside the local model domain at Forsmark intended for a deep geological repository for Sweden's spent nuclear fuel (SFK). The underpinning strategy of the protocol is that the integration of spatially distributed discrete and porous media flow modelling tools must be geologically (geometrically) conditioned and have at least one hydraulic calibration target in common. The geometrical conditioning and hydraulic calibration of the used flow modelling tools must be sufficiently consistent to ensure confidence regarding their usage in different hydrogeological applications, e.g., prediction of water table drawdowns during the construction of repository accesses, or prediction of post-closure groundwater fluxes between ground surface and repository depth including determination of exit locations in particle tracking simulations.

Notably, the design of the modelling protocol presented in this report is based on existing structural and hydraulic data from previous investigations in boreholes drilled from the ground surface. No additional surface-based boreholes are planned. Instead, new boreholes will be drilled and investigated from excavated underground openings to characterize the geometric and material properties of the bedrock adjacent to these openings at various depths. These new data will be critical for several modelling methodology reports under consideration by SKB for future site descriptions and safety assessments, as listed in Table 1-1 – particularly those concerning deterministic geological modelling (DGM) and discrete fracture network modelling (DFNMM).

Accordingly, it is expected that the modelling protocol presented in this report will be updated or revised to incorporate new structural models and hydraulic observations derived from these underground investigations. In other words, future versions of this methodology report (HGMM) will place greater emphasis on groundwater flow modelling within the Bedrock system.

A key element of the proposed protocol's workflow is its division into two stages: a DFN stage and an ECPM stage. This structure mirrors the approach used for groundwater flow modelling of the Bedrock system in SDM-Site (see Figure 5-1). In SDM-Site, hydraulic calibration in Step A was based on the DFN-2008 concepts, while Steps B through D applied ECPM concepts using hydraulic upscaling. It is important to note that the hydraulic calibration of the DFN model realizations in Step A incorporated deterministically modelled deformation zones and the subdivision of background fracturing into fracture domains but was otherwise geometrically unconditioned. The groundwater flow modelling protocol for the Bedrock system in SDM-Site also included paleoclimatic modelling (Step D in Figure 5-1). While this component is not included in the current modelling protocol presented in this methodology report, detailed information on the paleoclimatic modelling setup from SDM-Site is provided in Sections 2.6 and 2.7.2.

Since SDM-Site, the assumptions regarding initial hydrogeochemical conditions at 8000 BC have been further scrutinized. The initiation of paleoclimatic modelling now requires coordination with hydrogeochemical modelling to ensure conceptual consistency across disciplines (see Mercier et al. 2025).

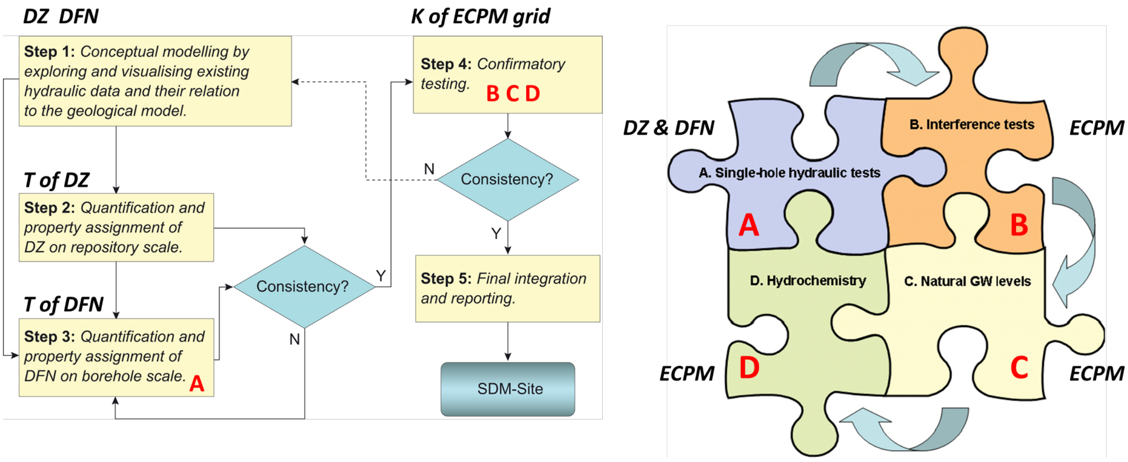

Figure 5-1. *Illustration of the protocol used for groundwater flow modelling of the Bedrock system in SDM-Site. The hydraulic calibration in Step A was based on DFN concepts and in Step B-D on ECPM concepts. Modified after Follin (2008).*

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