Technical Report

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Preliminary safety evaluation for the Simpevarp subarea

Based on data and site descriptions after the initial site investigation stage

Svensk Kärnbränslehantering AB

April 2005

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Preface

This report presents the preliminary safety evaluation of the Simpevarp subarea, based on data from SKB's initial site investigation stage at Simpevarp.

Johan Andersson, JA Streamflow AB has authored the report.

Comments have been provided by Jan-Olof Selroos, Ignasi Puigdomenech and Raymond Munier of SKB's safety assessment team on issues regarding hydrology/radionuclide transport, hydrogeochemistry and geology, respectively. The undersigned has provided the thermal calculations and the complementary calculation of the deposition hole exploitation ratio and associated text, as well as overall comments on the report.

The report has been reviewed by the following members of SKB's international Site Investigation Expert Review Group (SIERG): Per-Eric Ahlström, SKB (chair); Jordi Bruno Enviros, Spain; John Hudson, Rock Engineering Consultants, UK; Ivars Neretnieks Royal Institute of Technology, Sweden and Mike Thorne, Mike Thorne and Associates Ltd, UK.

Stockholm, April 2005

Allan Hedin
Project Leader

Summary

The main objectives of this Preliminary safety evaluation (PSE) of the Simpevarp subarea are: to determine, whether the feasibility study's judgement of the suitability of the candidate area with respect to long-term safety holds up in the light of the site investigation data; to provide feedback to continued site investigations and site-specific repository design and to identify site specific scenarios and geoscientific issues for further analyses.

The PSE focuses on comparing the attained knowledge of the sites with the suitability criteria as set out by SKB in /Andersson et al. 2000/. These criteria both concern properties of the site judged to be necessary for safety and engineering (requirements) and properties judged to be beneficial (preferences). The findings are then evaluated in order to provide feedback to continued investigations and design work. The PSE does not aim at comparing sites and does not assess compliance with safety and radiation protection criteria.

The evaluation shows that even considering remaining uncertainties, the Simpevarp subarea meets *all safety requirements* and *most of the safety preferences*. Consequently, from a safety point of view, there is no reason not to continue the Site Investigations of the Simpevarp subarea. There are still uncertainties to resolve and the safety would eventually need to be verified through a full safety assessment. Still, this Preliminary Safety Evaluation demonstrates that it is likely that a safe repository for spent nuclear fuel of the KBS-3 type could be constructed at the site.

There are uncertainties in the site description. However, this Preliminary Safety Evaluation shows that only some of these uncertainties have safety implications and would need further resolution. The following feedback is provided to the site investigations and the associated site modelling:

- Reducing the uncertainty on the deformation zone geometry within the Simpevarp subarea would allow for a more specified layout, although the sensitivity analysis shows that the space needed is rather robust with respect to uncertainties in the zones. However, if the complete site investigation programme was to focus on the Simpevarp subarea, there would be a need for more data from repository depth on potential repository volumes particularly north of the Simpevarp peninsula, but also in the southern parts of the subarea extending outside the current local model domain.
- There is substantial uncertainty in the discrete fracture network (DFN) model and this affects key safety aspects, like the probability of large fractures intersecting deposition holes, the upscaling of the hydraulic properties and the resulting transport resistance along migration paths from potentially breached canisters. Efforts need to be spent on reducing these uncertainties during the Site Investigation Phase both in terms of acquiring new data and from improved site modelling. It is especially important to provide robust estimates of the intensity of long fractures and features, e.g. the *k* parameter in the power law distribution being part of the DFN-model. Observations in the size interval that causes the discriminating fracture intersections, i.e. one to several hundred metres, are scarce. It is therefore desirable to increase the confidence in this interval of the size distributions.
- Current uncertainties in the stress regime and intact rock properties are sufficiently low from the construction point of view. Still, the issue of spalling due to the thermal load may require additional analyses, as already envisaged for the full safety assessment SR-Can. This may also lead to additional data demands.

- The thermal conductivity is relatively low and shows rather high and uncertain spatial variability. Unless these uncertainties are reduced, the design would need to consider relatively large canister separations in order to ensure that the temperature requirements on canister and buffer are met. Further reduction of uncertainties in the spatial variability and scaling of thermal conductivity would allow for a more compact design.
- Between 60 and 80 percent of blocks at the 20 m scale are estimated to have an effective hydraulic conductivity $K < 10^{-8}$ m/s. The rather high hydraulic conductivity, as well as the uncertainty in the spatial variation and upscaling warrant further studies.
- The groundwater composition meets all requirements and preferences, but further reduction of uncertainties would improve the arguments for assessing the future evolution of the groundwater composition.
- In order to evaluate the redox buffering capacity of the geosphere, detailed mineralogical data on Fe(II) and sulphide content of the rock and fracture minerals would be needed.
- The evaluation of flow-related transport parameters conducted with the regional groundwater flow model shows that both the preferences for Darcy velocity and the transport resistance F are met for almost all potential migration paths. However, the analysis has not been made with sufficient resolution for this conclusion to be robust and there are also substantial uncertainties with respect to the channelling of individual fractures. There is a need to reduce the uncertainties although this can only partly be achieved by new measurement approaches. Further attention to modelling, with different alternatives and careful scrutiny of assumptions, would elucidate the importance of these uncertainties.
- The migration properties of the rock matrix (porosity, formation factor and K_d) meet the preferred values. However, the values are based on few samples only and evaluation of more samples would thus enhance this conclusion.

The assessments made for the PSE also suggest some implications for design, some of which are of a generic character to be considered also for the other sites. The most important such feedbacks are:

- Compared to the actual safety requirement, the design rules for discarding canister positions due to potential intersection with too large fractures or deformation zones are overly restrictive. The percentage of deposition holes to be discarded would substantially decrease if the design rules were better harmonised with the actual safety requirements. However, it is important to note that current design rules overestimate the number of discarded deposition holes.
- The spatial variability of the thermal conductivity may be too large to be consistent with the currently adopted design rules, which only consider mean values and a margin to handle spatial variability. The additional temperature analyses conducted here and the predicted spatial variability of thermal conductivity imply that the canister spacing currently suggested by design may be insufficient at some canister locations. The temperature margin for the gaps between canister/buffer and buffer/rock and for the uncertainty/variability in rock thermal conductivity applied in the design work should be revisited, since the present rules seem to leave too little margin for these factors.

Finally, this PSE also highlights issues that would have to be considered if the Simpevarp subarea was to be assessed in a full safety assessment. Most of the issues are rather generic in nature and thus also warrant consideration in future safety assessments of other sites.

Sammanfattning

Målen för denna preliminära säkerhetsbedömning av delområde Simpevarp är att värdera om förstudiens bedömning om kandidatområdets lämplighet ur säkerhetssynpunkt kvarstår i ljuset av nu tillgängliga platsundersökningsdata, att ge återkoppling till de fortsatta platsundersökningarna och arbetet med förvarsutformningen samt att identifiera platsspecifika scenarier och geovetenskapliga frågeställningar som kan behöva belysas i det fortsatta arbetet.

Säkerhetsbedömningen innebär främst att erhållen kunskap om platsen jämförs med de lämplighetsindikatorer som SKB tidigare har presenterat /Andersson et al. 2000/. Kriterierna avser dels platsegenskaper som bedömts nödvändiga för säkerhet och projektering (krav) och platsegenskaper som bedömts vara fördelaktiga (önskemål). Resultatet av jämförelsen värderas sedan för att ge återkoppling till de fortsatta platsundersökningarna och projekteringsarbetet. Säkerhetsbedömningen innefattar inte att jämföra platser och det sker ingen direkt värdering om ett förvar på platsen uppfyller ställda krav på säkerhet och strålskydd.

Den gjorda utvärderingen visar, trots kvarvarande osäkerheter, att delområde Simpevarp *uppfyller alla krav* och *de flesta av önskemålen*. Från säkerhetssynpunkt finns det därför ingen anledning att inte fortsätta platsundersökningarna i delområde Simpevarp. Det finns dock kvarvarande osäkerheter och om ett förvar skulle lokaliseras till delområdet behöver säkerheten verifieras i en fullständig säkerhetsanalys. Den preliminära säkerhetsvärderingen visar dock att det är troligt att ett säkert KBS-3-förvar för använt kärnbränsle kan förläggas till delområdet.

Det finns osäkerheter i platsbeskrivningen, men den preliminära säkerhetsbedömningen visar att det bara är en del av dessa osäkerheter som har betydelse för säkerheten och som ur denna aspekt skulle behöva reduceras. Följande återkoppling görs till platsundersökning och tillhörande platsmodellering:

- Genom att minska osäkerheterna i geometrin for deformationszonerna i delområde Simpevarp skulle en mer precis förvarslayout kunna tas fram, även om gjorda känslighetsstudier visar att den nödvändiga förvarsvolymen inte påverkas så mycket av osäkerheter i denna geometri. Om den kompletta platsundersökningen skulle fokusera på delområde Simpevarp, skulle det dock behövas mycket mer data från förvarsdjup speciellt norr om Simpevarpshalvön, men även i de södra delar som ligger utanför det nu gällande lokala modellområdet.
- Osäkerheterna i den diskreta spricknärverksmodelleringen (DFN) är betydande och dessa påverkar centrala säkerhetsaspekter, som sannolikheten för att stora sprickor korsar deponeringshål, uppskalning av hydrauliska egenskaper och resulterande transportmotstånd längs transportvägar från eventuellt skadade kapslar. Insatser behövs för att minska dessa osäkerheter, både insamlande av ytterligare data och förbättrad platsmodellering. Det är speciellt viktigt att ta fram robusta skattningar av intensiteten av långa sprickor, dvs. den s.k. k-parametern i den fördelningsfunktion som används i DFN-modelleringen. Det finns idag få observationer i det storleksintervall av sprickor som inte bör korsa deponeringshål, dvs. från hundra till några hundra meter. Det är därför angeläget att öka tilltron i just detta intervall i storleksfördelningen.

- Osäkerheter för bergspänningar och det intakta bergets mekaniska egenskaper bedöms vara tillräckligt små för att bygga förvaret. Frågan om den termiska lasten från det använda bränslet skulle kunna ge upphov till uppsprickning i en del deponeringshål kan dock behöva värderas, vilket också kommer att ske inom ramen för säkerhetsanalysen SR-Can. Resultaten av dessa värderingar skulle kunna leda till ytterligare databehov.
- Den termiska ledningsförmågan är relativt låg och uppvisar även ganska stor och osäker rumslig variation. Om inte dessa osäkerheter minskas behövs en förvarsutformning med relativt stora kapselavstånd för att försäkra att temperaturkrav på kapselyta och buffert klaras. Ytterligare reducering av osäkerheterna i den rumsliga variationen skulle tillåta en mer kompakt layout.
- Mellan 60 och 80 procent av alla block i 20 m skala uppskattas ha en effektiv hydraulisk konduktivitet $K < 10^{-8}$ m/s. Denna relativt höga hydrauliska konduktivitet, såväl som osäkerheterna i den rumsliga variationen behöver studeras ytterligare.
- Grundvattnets sammansättning uppfyller både ställda krav och önskemål, men ytterligare reducering av osäkerheterna skulle förstärka argumentationen om sammansättningens utveckling i framtiden.
- För att bedöma geosfärens kapacitet för redoxbuffring behövs detaljerade mineralogiska data om Fe(II) och sulfidinnehåll i berget och i sprickmineralen.
- De flödesrelaterade transportparametrar som beräknats med den regionala grundvatte nflödesmodellen visar att både önskemålen för darcyhastighet och transportmotstånd F uppfylls för nästan alla tänkbara transportvägar. Beräkningen har dock inte gjorts med tillräcklig upplösning och det finns även betydande osäkerheter t ex beträffande kanalbildning inom enskilda sprickor, vilket gör bedömningen mindre robust. Det finns ett behov av att minska osäkerheterna även om detta bara delvis kan göras med hjälp av ytterligare platsdata. Ytterligare fokusering på modellering, med olika alternativ och noggrann analys av gjorda antaganden behövs.
- Bergmatrisens transportegenskaper (porositet, formationsfaktor och K_d) uppfyller önskemålen. Angivna värden bygger dock på ett fåtal prov och en analys av fler prov skulle förstärka slutsatsen.

Den preliminära säkerhetsbedömningen drar också några slutsatser av betydelse för det fortsatta designarbetet. En del av dessa slutsatser är allmänna och har därför betydelse även för de andra platserna som nu studeras. De viktigaste av dessa är:

- Jämfört med de faktiska säkerhetskraven är projekteringens regler för att utesluta deponeringshål på grund av att de korsar för stora sprickor för restriktiv. Andelen deponeringshål som skulle behöva uteslutas skulle minska väsentligt om designreglerna bättre harmoniserades med de faktiska säkerhetskraven. Å andra sidan är det viktigt att konstatera att projekteringen idag överdriver, och inte underskattar, antalet deponeringshål som skulle behöva uteslutas av detta skäl.
- Värmeledningsförmågans rumsliga variation tycks vara för stor för att inneslutas i de marginaler som nu används som designregel. Kompletterande termiska analyser genomförda i denna rapport antyder att nu föreslaget avstånd mellan kapslar inte är tillräckligt för vissa kapselpositioner. Antagna marginaler för temperatursprånget i gapen mellan kapsel/buffert och buffert/berg bör åter värderas, eftersom nuvarande designregel tycks lämna för liten marginal för dessa faktorer.

Den preliminära säkerhetsvärderingen uppmärksammar slutligen ett antal frågeställningar som behöver beaktas om delområde Simpevarp skulle analyseras i en full säkerhetsanalys. De flesta av dessa frågeställningar är av generisk natur och bör därför även beaktas för andra platser.

Contents

1 Introduction

This report is a Preliminary Safety Evaluation (PSE) of the Simpevarp subarea being investigated by SKB. Similar evaluations will be conducted for the Forsmark area and the Laxemar subarea.

1.1 Purpose and objectives

Radioactive waste from nuclear power plants in Sweden is managed by the Swedish Nuclear Fuel and Waste Management Co, SKB. Systems are already in place for handling operational waste and for transporting and storing the spent nuclear fuel. The two principal remaining tasks in the programme are to locate, build and operate i) an encapsulation plant in which the spent fuel will be emplaced in canisters and ii) i) a deep repository where the canisters will be deposited. For this reason, SKB pursues site investigations for the deep repository in the municipalities of Östhammar, the Forsmark area, and Oskarshamn. In Oskarshamn, the area is divided into two parts, the Simpevarp subarea, concentrated on the Simpevarp Peninsula and the Laxemar subarea located on the mainland west of the Simpevarp Peninsula, see Figure 1-1.

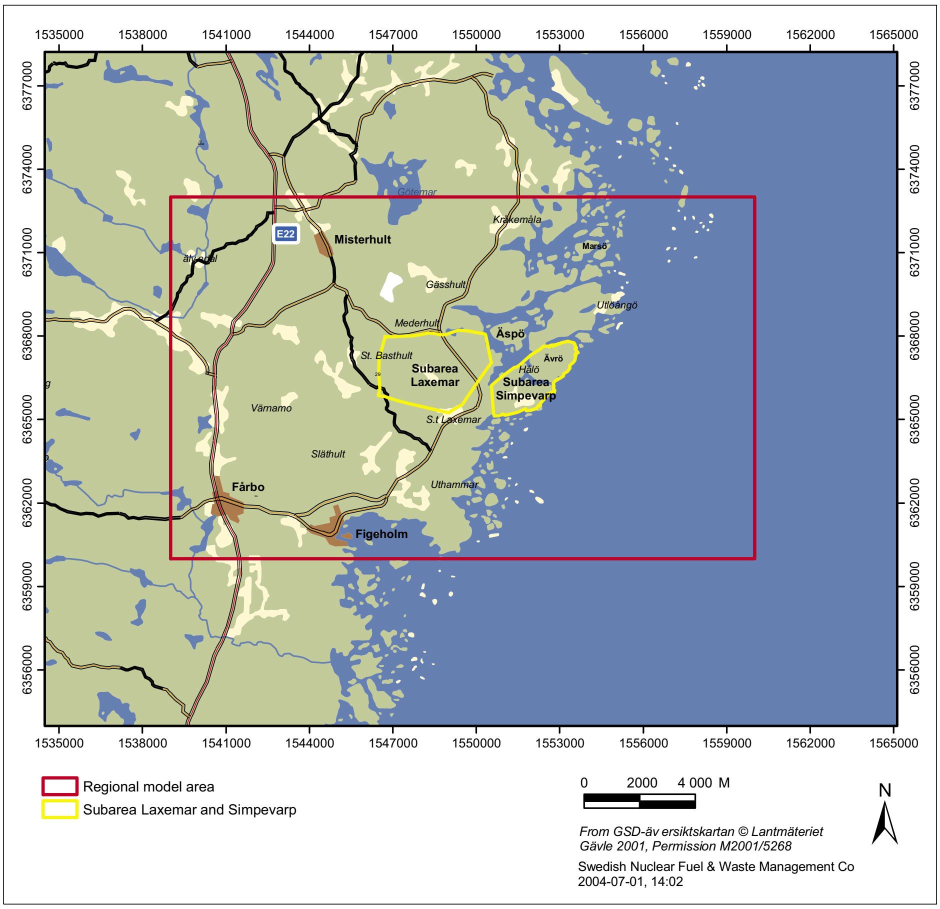

Figure 1-1. Overview of the Simpevarp area and identification of the Simpevarp and Laxemar subareas (Figure 1-2 of SDM S1.2).

The investigations /SKB, 2001/ are carried out in two stages, an initial investigation followed by a complete investigation, should the results after the initial stage be favourable. A preliminary safety evaluation, PSE, is made at the end of the initial stage, based on available field data and preliminary layouts for the deep repository at that stage. Separate preliminary safety evaluation reports are planned for Simpevarp, Forsmark and Laxemar.

The main objectives of the evaluation are:

- to determine whether the feasibility study's judgement on the suitability of the candidate area with respect to long-term safety holds up in the light of the findings from the site investigation,
- to provide feed-back to continued site investigations and site-specific repository design and
- to identify site specific scenarios and geoscientific issues for further analyses.

The PSE is concerned with site suitability with respect to radiological long-term safety. It does not aim at comparing sites and does not assess compliance with safety and radiation protection criteria. Environmental effects due to the construction and operation of the repository will be addressed in the environmental impact assessment and are not discussed in this document.

1.2 Overview of methodology

In order to meet the objectives, the PSE focuses on comparing the attained knowledge of the sites to the suitability criteria as set out by SKB in /Andersson et al. 2000/. Some of these criteria are absolute requirements whereas others are preferable conditions that would influence safety in a positive manner. The criteria are formulated for different subject areas, i.e. geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry and radionuclide transport.

The assessment, presented in Chapter 3, follows these subject areas. First the criteria are presented, but it is also considered whether these criteria would need to be modified due to findings or design changes made since the issue of the criteria. After presenting the criteria and the additional considerations, the relevant findings from the Site Modelling /SKB, 2005a/ and the design work /SKB, 2005b/ are presented. Usually these analyses are sufficient to address the performance relative to the criteria, but in some instances some additional calculations, performed directly by the Safety Assessment team are added. After presenting all these results, there is an evaluation of the degree to which the criteria and additional considerations are fulfilled with respect to safety and what feedback may be given to the further site investigation and repository design work.

1.3 Developments since the planning document and implications for the PSE

Since the issuing of the PSE planning document, SKB's Safety Assessment planning has evolved and relationships between activities related to site investigations and safety assessments have been further detailed. Two reports on long-term safety, SR-Can and SR-Site, will be produced in 2006 and 2008, respectively. SR-Site will support the application to build a deep repository. SR-Can is a preliminary version of SR-Site and will provide feedback to continued site investigations. It will also allow the Swedish authorities to comment on SKB's methodology for safety assessments before it is used in support of a licence application. SR-Can will be based on site data from the initial site investigation phase and SR-Site on data from the complete site investigation. An interim version of SR-Can /SKB, 2004b/ is already published.

According to the current prerequisites for planning, the complete site investigations will concern the Forsmark and Laxemar areas and both SR-Can and SR-Site will consequently consider repositories located in these two areas. The main reasons, currently envisaged, for setting aside the Simpevarp subarea are flexibility and space considerations. Available underground space for a deep repository is expected to be limited at the Simpevarp subarea in comparison to the two other candidate areas. A definite decision on what subarea to prioritize in Oskarshamn will be taken when data from the Simpevarp area, including this preliminary safety evaluation, have been evaluated.

An objective of SR-Can is to preliminarily assess the safety of the two sites given the descriptions of the canisters to be produced in the encapsulation plant and the host rock conditions at the sites in so far as they can be specified after the preliminary site investigation phase. The intention is not to fully establish the suitability of the studied sites – this will be done in SR-Site. The intention is also not to finally establish the technical system for disposal – but rather to investigate the safety of the system as it is specified at that stage, and to give feedback for the further development. It is important already at the time of SR-Can to have established the likely viability of disposal at one or more of the sites.

Preliminary Safety Evaluations are being made for all sites, i.e. including the Simpevarp sub-area. The evaluations are made as sub-tasks within the SR-Can project. However, some of the analyses envisaged in the PSE planning document /SKB, 2002a/ will now appear as either sub-tasks in SR-Can or as part of Site Descriptive Modelling or Repository Engineering activities, see further section 3.1. The implications of this is discussed in section 3.8, but it can generally be stated that the combination of the current level of PSE with the more detailed evaluation in SR-Can implies a more thorough evaluation of findings of the initial site investigations than originally envisaged.

1.4 INSITE review of PSE planning document

The PSE planning document /SKB, 2002a/ has been reviewed by the SKI international review group INSITE /SKI, 2004/. The following main points were brought up in the review:

- The review states that "In general, the level of analysis planned for the PSE is what would be expected at this stage of a site investigation project, although there are some issues for discussion".
- The reviewers express concern that the result of the PSE would arrive too late to impact the setup of the Complete Site Investigation Phase.
- The respective roles of the PSE and the then envisaged limited safety assessment SR-Met was judged unclear by the reviewers.
- The reviewers expressed a need to also assess the impact of thermal buoyancy effects, i.e. flow caused by the heat generation from the spent nuclear fuel, and to assess the potential development and significance of an Excavation Disturbed Zone (EDZ).

The reviewers also make some more detailed comments and suggestions. Most of the suggested additions will be addressed in SR-Can (and the subsequent SR-Site) rather than in the PSE.

In response to these views, it should be noted that the PSE is not the sole form of feedback to the Site Investigation activities. Several individuals from the SR-Can team are e.g. deeply involved in the site modelling from which much feedback to the Site Investigations is given. Furthermore, a formal check of the Complete Site Investigation (CSI) programme will be made after each completed PSE which will allow for adding complementary investigation activities for the later data freezes of the CSI, if such are judged to be needed.

The SKB plans for Safety Assessments have evolved and the limited in scope SR-Met is now replaced by the full Safety Assessment SR-Can. Its role and relation to PSE are described in the next section.

Thermal buoyancy is not judged to be of significant importance to safety, see e.g. the SR 97 Process report /SKB, 1999a/. Furthermore, the need to consider thermal buoyancy will be re-assessed in the SR-Can (and SR-Site) Process Reports. The development and properties of the EDZ will be addressed in SR-Can and updated in SR-Site.

2 Basis for the safety evaluation

This chapter provides reference to the Site Descriptive Model of the Simpevarp subarea and to the engineering work that has been applied in order develop a preliminary repository design. This input is used in the evaluation presented in Chapter 3.

2.1 Site descriptive model

The preliminary site description of the Simpevarp subarea version 1.2, /SKB, 2005a/ and denoted SDM S1.2 in this document, is based on the field data collected during the initial site investigation phase. Also, the findings from the earlier versions of the site description, namely SDM S1.1 /SKB, 2004b/ and version 0 /SKB, 2002b/, are incorporated in model version 1.2. The site descriptive model is presented on a local and a regional scale, see Figure 2-1, with an accompanying synthesis of the current understanding of the site.

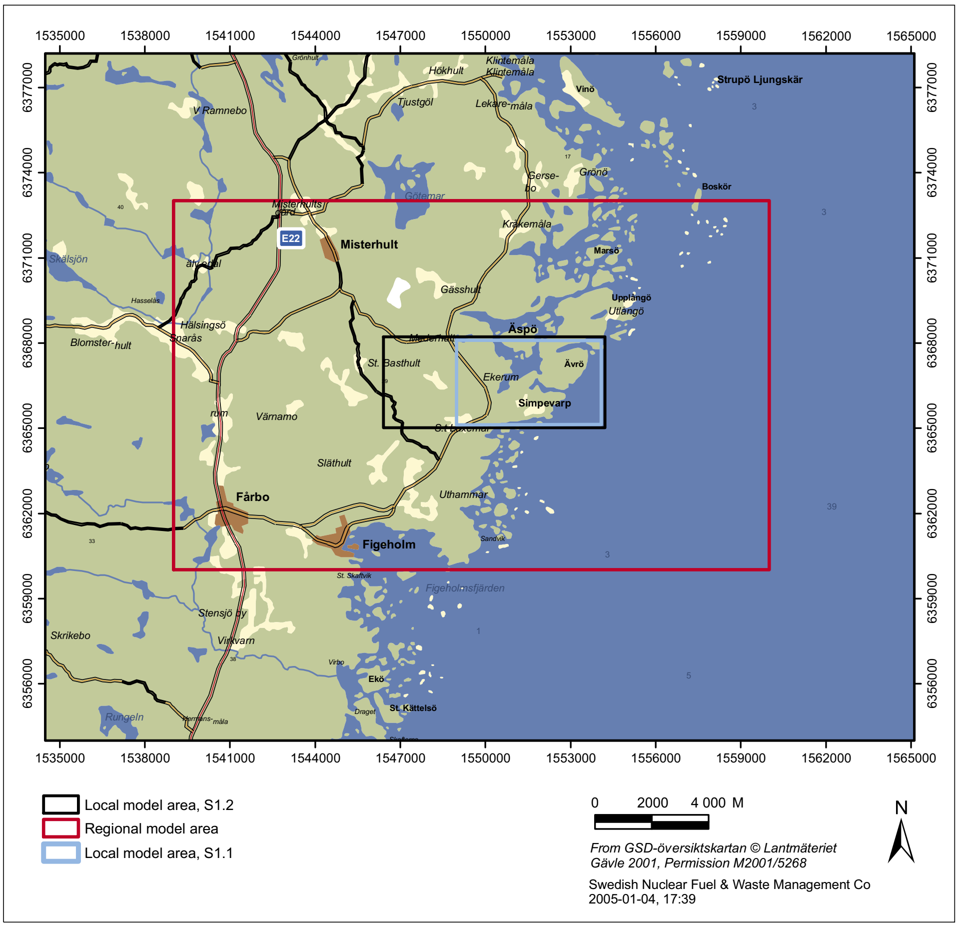

Figure 2-1. *Regional and local model areas, Figure 2-3 in SDM S1.2.*

2.1.1 Investigations and available data

The Simpevarp area, which includes the Simpevarp and Laxemar subareas as seen in Figure 1-1, is located in the province of Småland, County of Kalmar, within the municipality of Oskarshamn, and immediately adjacent to the Oskarshamn nuclear power plant (OI–OIII) and the Central interim storage facility for spent fuel (Clab I and Clab II). The Simpevarp area is located close to the shoreline of the Baltic Sea. The easternmost part (Simpevarp subarea) includes the Simpevarp peninsula (which hosts the power plants and the interim storage facility for spent fuel (Clab)) and the islands Hålö and Ävrö. The island of Äspö, under which the Äspö Hard Rock Laboratory (Äspö HRL) is developed, is located some two kilometres north of the Simpevarp peninsula. The areal size of the Simevarp subarea is approximately 6.6 km^2, whereas the Laxemar subarea covers some 12.5 km^2.

Investigations have been in progress in the Simpevarp subarea from about March 2002. The data freeze for the Simpevarp 1.1 model version was set at July 1, 2003 and reported in the version S1.1 Site Descriptive Report /SKB, 2004b/. The data freeze for SMD S1.2 was set at April 1, 2004.

The surface investigations undertaken in the Simpevarp subarea comprise airborne photography, airborne and surface geophysical investigations, lithological mapping of the rock surface, mapping of structural characteristics, mapping of Quaternary deposits and soils, marine geological investigations, hydrogeochemical sampling and analysis of surface waters and various surface ecological inventory compilations and investigations. The drilling activities during this time comprised:

- Four approximately 1,000 m deep cored boreholes and two 100 m cored boreholes in the immediate vicinity of two of the deep holes. To this should also be added borehole KLX04 drilled in the Laxemar subarea (from which only limited investigation data, e.g. stress measurements, were available for the SDM S1.2).
- Three percussion-drilled boreholes with lengths ranging up to 200 m and reaching vertical depths of 185–200 m.
- Soil/rock drilling of 19 boreholes, including four boreholes drilled for environmental monitoring in conjunction with the drill sites on the Simpevarp peninsula.

The borehole investigations performed following the drilling of the boreholes can broadly be divided into logging, detailed mapping, rock stress measurements, hydraulic measurements, sampling of rock and fractures for determination of density, porosity, susceptibility, mineralogy, geochemistry, diffusivity, sorption properties, rock strength and thermal properties, and groundwater sampling for the hydrogeochemical analyses. All data are stored in the SKB databases SICADA and SKB GIS. The basic primary data are also described in the SKB P-series of reports. In addition to the new data, there has also been a review of old data from Äspö and data from the construction of the nuclear power plants and the Clab facility. Full references to the P-reports and a more detailed description of the database are given in SDM S1.2.

2.1.2 The site descriptive model report

In the Site Descriptive Modelling, data are first evaluated within each discipline and the evaluations are then synthesised between disciplines. Three-dimensional modelling, with the purpose of estimating the distribution of parameter values in space, as well as their uncertainties, follows. The geometrical framework for modelling is taken from the geological model, and is subsequently used in rock mechanics, thermal, hydrogeological and hydrogeochemical modelling. The three-dimensional description presents the parameters with their spatial variability over a relevant and specified scale, with the uncertainty included in this description. If required, different alternative descriptions are provided.

The Site Descriptive Model Report, see SDM S1.2, first summarises available primary data and provide an overview of their usage and then describes the development of the geosphere and the surface systems in an evolutionary perspective. Subsequent chapters in SDM S1.2 (Chapters 4 to 10) set out the modelling of surface ecology, geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry and transport properties, respectively. Each chapter provides the discipline-based accounts of evaluation of the primary data, three-dimensional modelling and discussion of identified uncertainties associated with the developed models. Chapter 11 presents the resulting descriptive model of the Simpevarp subarea in a condensed form. Chapter 12 assess overall consistency and confidence in the description. Chapter 13 provides the overall conclusions of the work.

2.1.3 Overall confidence in the modelling

The understanding of the Simpevarp subarea is addressed and discussed in Chapter 12 of the SDM S1.2 where also the identified uncertainties of the developed discipline models are articulated and an overall confidence assessment is provided in the light of model interactions and integration. Chapter 13 sets forth tentative conclusions about the general understanding of the Simpevarp subarea.

Overall uncertainties and confidence

Despite all data being available for analysis, there is still uncertainty associated with the description of the Simpevarp subarea in the SDM S1.2. However, important modelling steps have been taken and the main uncertainties are identified, in some cases quantified, or explored as alternatives. There are however some uncertainties that remain unquantified at this stage and where the alternative hypotheses formulated have not been developed into models. The uncertainties of relevance to the PSE are presented and discussed in Chapter 3 below.

Also, the possible interactions between disciplines, and the interactions considered for SDM S1.2 are assessed. It is obvious that changes to the lithological model have a strong impact on most disciplines (e.g. rock mechanics, thermal and transport properties). The deformation zone model in particular influences the hydrogeological and rock mechanics models. Likewise, there is a strong interdependence between hydrogeology and hydrogeochemistry, primarily through the description of mixing, proposed as being mainly responsible for the evolution of the groundwater chemistry, including the distribution of salinity over time. The hydrogeochemical model in turn is to a limited degree dependent on the chemical composition of the bedrock and the fracture minerals. The sorption characteristics in the transport model depend on geology (mineralogy) and hydrogeochemistry (the groundwater composition). Other couplings to consider in the transport model are rock stress effects, both in virgin rock (in the vicinity of boreholes) and in drill core rock samples (effects of unloading of rock stresses on laboratory results), on anisotropy in diffusion properties, possibly associated with any existing fabric (foliation) of the bedrock. Many interactions are evident within the surface system, and this is also the reason for integrating the surface analyses. The interactions between the surface system and the bedrock system remains to be better established and quantified. This applies primarily to the turnover of water and chemical mass balances. There is also an interest in quantifying how these turnovers and mass balances are influenced by changing climatic and landform characteristics.

The need for geology to provide input to other disciplines has guided the setup of the geological modelling, as further discussed in the general execution programme for the Site Investigations /SKB, 2001/, but in preparing the SDM S1.2, it was not possible to take into account all feedbacks from rock mechanics, hydrogeology and hydrogeochemistry models to geological modelling. The basis for such evaluations and transfers is expected to be significantly improved in the subsequent Laxemar 1.2 geological modelling. Of particular interest in this context is evidence of hydraulic connections, as indicated from drilling and/or cross-hole interference test pressure responses. These could potentially help assess the hydraulic properties and connectivity (and extent) of certain interpreted deformation zones. This analysis requires boreholes equipped with packer systems and pressure transducers and appropriate distances between boreholes, and the possibility of resolving hydraulic disturbances of a magnitude commensurate with the level of hydraulic conductivity and connectivity of interest.

The Simpevarp 1.2 site descriptive model is in general agreement with current understanding of the past evolution of the area. This applies e.g. to the composition of present groundwater in relation to the bedrock lithology and fracture mineralogy. Furthermore, the hydrogeological modelling of groundwater chemical evolution does not contradict the groundwater compositions assessed from the borehole data. It is identified as potentially interesting to analyse and improve the understanding of the relation between geological evolution, including formation of different fracture sets, with (hydro-)geochemical indicators (including fracture minerals). No major surprises have been noted in the Simpevarp 1.2 modelling.

Current status of important site-specific questions

In the execution programme for the Simpevarp area /SKB, 2002c/, a number of important site-specific questions were formulated. They concerned "Size and locations of rock volumes with suitable properties, location and importance (particularly in terms of permeability) of fine-grained granite bodies and fracture zones, high rock stresses, thermal conductivity of the bedrock, rock mechanics properties of rock mass, and ore potential".

Based on the outcome of the Simpevarp 1.2 modelling the current status on these questions can be reported as follows:

- *"Size and locations of rock volumes with suitable properties (Simpevarp peninsula)":* Uncertainty in the deformation zone model still persists, but is primarily related to the interpreted "possible" zones (of low or intermediate confidence of occurrence) mainly located in, the volumes northwest of deformation zone ZSMNE012A, the neighbouring Laxemar subarea and in the regional scale model volume.
- *"Location and importance (particularly in terms of permeability) of fine-grained granite and fracture zones":* Fine-grained granite and pegmatite veins and dikes exist throughout the investigated Simpevarp subarea. There is limited new information on material properties of the interpreted deformation zones as obtained from borehole intercepts with the zones.
- *"High rock stresses"* do not appear to be a major concern for the Simevarp area. The current stress model indicates lower stresses in the Simpevarp subarea east of deformation zone ZSMNE012A, attributed to unloading controlled by the geometry of existing deformation zones, compared with the area west thereof.
- For the description of *"rock mechanics properties of the rock mass"*, laboratory data are underpinned by empirical and theoretical relationships, the former making indirect inferences using empirical relationships based on the Q and RMR indices and the latter approach makes use of simulated loading tests in a developed DFN model.

- The analysis of the *"thermal conductivity"* indicates that the thermal conductivity in the Simpevarp subarea generally is low. A methodology for upscaling of thermal conductivity data has also been developed.
- The *"ore potential"* has been assessed by an independent exploration company /Lindroos, 2004/. The ore potential is considered negligible, with a real potential only for quarrying of building- and ornamental stone associated with the Götemar and Uthammar granite intrusions to the north and south of the investigated area, respectively.

Overall, the remaining issues specific to the Simpevarp subarea following the Simpevarp 1.2 modelling are primarily associated with detailing the descriptions of geological, thermal, mechanics, hydrogeological and hydrogeochemical properties at depth. In addition, the description of geometry and properties of important deformation zones in the Simpevarp subarea, some of which are repository volume-delineating zones, could be substantiated by more (borehole) data to assess heterogeneity and provide a statistical description of properties. However, it is not practically feasible to verify all possible zones by new boreholes or excavation trenches. Neither is this needed from a safety assessment point of view. The details of the deformation zones in the regional domain, outside the Simpevarp subarea have limited impact on flow and hydrogeochemistry in the potential repository volume.

2.2 Preliminary layout

The design premises and methodology for application in the preliminary design of underground excavations within the framework of SKB's site investigations is presented in "Deep Repository: Underground Design Premises. Edition D1/1", /SKB, 2004c/. According to these design premises the goals of the design work during the Complete Site Investigations (CSI) are to:

- Present a facility description for the chosen site with a proposed layout for the deep repository facility's surface and underground parts as a part of the supporting material for an application. The description shall present constructability, technical risks, costs, environmental impact and the reliability and effectiveness of the operational phase. The underground layout shall be based on information from the CSI phase and serves as a basis for the safety assessment.
- Provide a basis for the Environmental Impact Assessment (EIA) and consultation regarding the site of the deep repository facility's surface and underground parts with proposed final locations of ramp and shafts, plus the environmental impact of construction and operation.
- Carry out the design work for the entire deep repository facility to the point that it is possible to plan for the construction phase. SKB shall also show/explain what technical solutions do not need to be engineered in detail in this phase.

Ultimately, the design work should lead to a layout D2, to be used in the application for the Deep Repository, which will be submitted after the CSI. An intermediate step in the design work is to carry out design step D1 after the Initial Site Investigation.

2.2.1 Methodology

For the design step D1 a design methodology is developed in the design premises document /SKB, 2004c/. This is applied to each site. The design methodology aims at addressing several design tasks. Each task addresses a design issue. In a first step the following issues and tasks are addressed:

A: What locations and depths within the site may be suitable for locating the deep repository?

B: Is it reasonable to consider that the repository volume can be accommodated, taking into account current respect distances to deformation zones and preliminary assumed losses of deposition holes?

C: How can the deposition areas be designed with a view towards achieving sufficient space and long-term safety? With the sub-issues:

- C1. How can deposition tunnels, deposition holes and main tunnels be designed considering the equipment and the activities they are required to accommodate.
- C2. What distance may be required between deposition tunnels and between deposition holes in order to conform with the maximum permissible temperature on the canister surface?
- C3. What orientation may be suitable for deposition tunnels taking into account both water seepage and stability in deposition tunnels and deposition holes?
- C4. How large a proportion of the deposition holes may be unusable based on the minimum permissible distance to fractures or fracture zones of too large size, excessive water inflow and instability? How is the loss affected by different criteria rejection?
- C5. At what depth or over what depth range may it be suitable to build the deep repository? Is there a site-specific depth dependence?

D: How can other underground openings, especially the central area's rock caverns, be designed to achieve stability and to accommodate the required equipment and activities?

E: How can the layout of the entire hard rock facility be configured?

The answers to these questions also have potential safety implications since the issues to be solved by the Rock Engineering team to a large extent concerns adapting the layout in order to meet safety requirements and preferences.

Subsequent steps in the D1 design work concern engineering implications of the suggested design, like estimates of potential upconing and grouting needs. Also these issues could have some safety implications, but assessing this is not part of the PSE, as further discussed in section 3.8.

2.2.2 Applying the methodology to the Simpevarp subarea

A type D1 design has been developed for the Simpevarp subarea, see Figure 2-2, and reported in /SKB, 2005b/. It should be noted that the assessed area extends to a limited extent to the south of the local model area in the SDM S1.2. The bounds of the subarea are motivated by the location of bounding deformation zones and administrative restrictions.

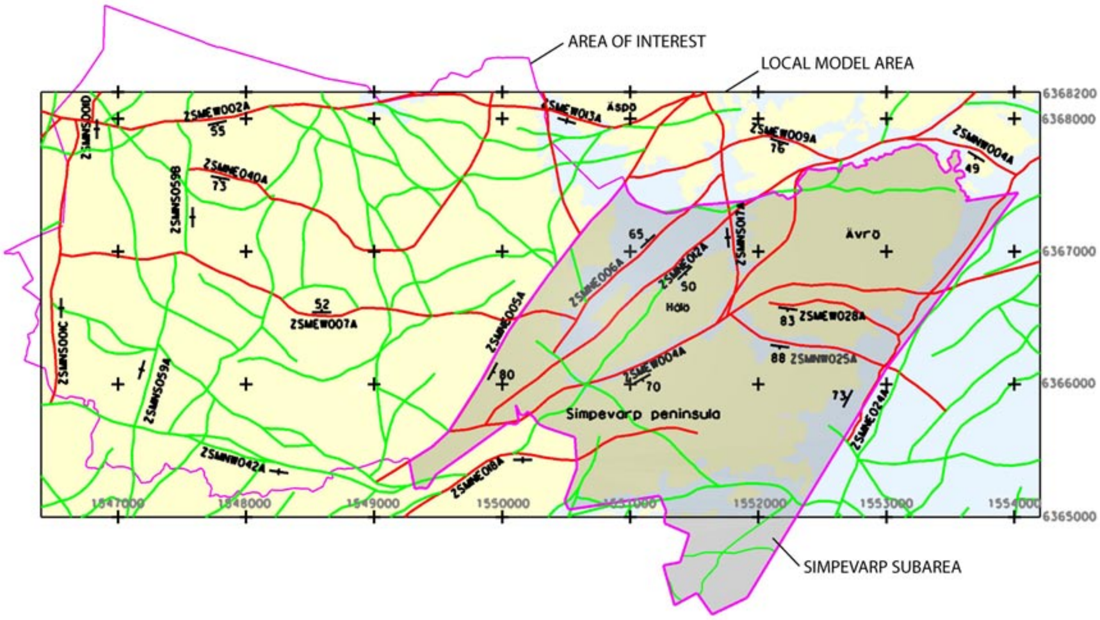

Figure 2-2. *The local model area and the area assessed in the Rock Engineering layout work (grey shaded). The latter essentially coincides with the Simpavarp subarea. Red and green lines are the surface intersections of modelled deformation zones, see section 3.2.4. (From /SKB, 2005b/).*

The design considers a repository for 4,500 canisters, based on current estimates of the final amount of spent fuel being produced in Sweden, but also assesses the space needed for an additional 1,500 canisters in case the final amount of spent nuclear fuel should supersede current estimates. Layouts are presented both for the –400 m and –500 m levels – the latter is the reference option. The possibility to adapt the layout to the interpreted deformation zones and the findings of the assessments addressing question C, are presented and discussed in Chapter 3 of this PSE.

3 Analyses and comparison to criteria

This chapter summarises the analyses of the site data forming the basis for the PSE. These analyses have mostly been conducted within the Site Descriptive Modelling and the subsequent Rock Engineering design work and are fully described in associated reports.

3.1 Overview and means of evaluation

The PSE planning document identified a set of analyses to be undertaken in order to meet the objectives of the evaluation, i.e. to allow comparison with criteria and to provide feedback to Site Investigations and Rock Engineering. Most of these analyses have been conducted as a part of the Site Descriptive Modelling SDM S1.2 /SKB, 2005a/ and the subsequent Rock Engineering exercise /SKB, 2005b/. The subsequent sections in this chapter summarise the main findings of these analyses.

3.1.1 Analyses considered in the PSE

Table 3-1 gives an overview of analyses used as a basis for the PSE. The table also makes on overview of analyses to be carried out in SR-Can and SR-Site, although these analyses will not be made for the Simpevarp sub-area according to current planning, see section 1.3. In the planning document for the PSE, additional analyses, designed to provide further feedback to the continued investigations and site-specific repository design were envisaged. Omitting these analyses is judged to have negligible impact on the PSE, although the analyses are important, and should be carried out eventually, as further discussed in section 3.8.

Table 3-1. Safety related geosphere and biosphere analyses at various stages of the site investigation. The abbreviations in the columns indicate which of the three project groups involved in the site investigation will be responsible for the analysis; Site Descriptive Modelling (SDM), Repository Engineering (RE) or Safety Assessment (SA).

Type of analysis	PSE	SR-Can	SR-Site
Thermal analyses			
Thermal evolution of canister surface, buffer and near field rock			
– for present climate conditions	RE, SA	RE, SA	RE, SA
– for future climate conditions	No	SA	SA
Thermal evolution at the site scale			
– for present climate conditions	No	SA	SA
– for future climate conditions	No	SA	SA
Hydraulic analyses			
Groundwater flow calculations (and salinity evolution) at superregional, regional and local scales			
– for historic conditions	SDM	SDM	SDM
– for present climate conditions	SDM	SDM	SDM
– for future climate conditions	No	SA	SA

Type of analysis	PSE	SR-Can	SR-Site
Particle tracking for t_w, F and discharge point distribution in the flow field			
– for present climate conditions	Based on regional model and simplified layout	SA, for layout according to D1 and using higher resolution	SA
– for future climate conditions	No	SA	SA
Drawdown and upconing analyses	No	RE, SA	RE, SA
Resaturation	No	RE, SE	RE, SA
Mechanical analyses			
Thermally induced rock stresses, considering inhomogeneous thermal rock properties	No	SA	RE/SA
Mechanical stability during construction and operation	RE	RE/SA	RE/SA
Earthquake analyses, all time frames	Assessment of probability of deposition hole with radius > 100 m; RE, SA	SA	SA
Long-term stability, effects of glacial load, ridge push etc.	No	SA	SA
Chemical analyses			
Groundwater chemical evolution inlcuding colloids			
– historic and initial state	SDM	SDM	SDM
– future evolution (different scenarios)	No	SA	SA
Chemical evolution of buffer and canister	No	SA	SA
Backfill chemical evolution	No	SA	SA
Radionuclide speciation calculations	No	SA	SA
Assessment of ore potential	SDM	SDM	SDM
Influence of construction materials etc	No	SA	SA
Radionuclide transport analyses (geosphere)			
Transmission calculations and transport modelling			
– for present climate conditions	No	SA	SA
– for future climate conditions	No	SA	SA
Colloid facilitated transport	No	SA	SA
Biosphere analyses			
Near- surface hydrology			
– for present conditions	SDM	SDM	SDM
– for future climate conditions	No	SA	SA
Biosphere model for radionuclide transport			
– for present conditions	No	SA	SA
– for future climate conditions	No	SA	SA
Dose and risk calculations	No	SA	SA

3.1.2 Means of comparision

SKB has established criteria with which the properties of a candidate host rock will be compared /Andersson et al. 2000/. Some of these are absolute requirements whereas others are preferable conditions that would influence safety in a positive manner. The criteria are based on the state of knowledge and the repository design plans at the time when the criteria were formulated.

/Andersson et al. 2000/ also noted that new R&D results and/or a modified basic repository design could motivate modifications of the criteria. For the purpose of this PSE, the criteria are still generally judged applicable. However, in some areas the knowledge base has expanded. Therefore, after shortly presenting the previous preferences and criteria for each subject area there is also a subsection providing conclusions from such additional considerations – if any. These additional considerations usually concern more specific/ quantified rules or minor modifications of the previous criteria.

The assessment is made for each subject area, i.e. geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry and transport, following the outline of /Andersson et al. 2000/. After presenting the criteria and the additional considerations, the relevant findings from the Site Modelling /SKB, 2005a/ and the design work /SKB, 2005b/ are presented. Usually these analyses are sufficient to address the performance relative to the criteria, but in some instances some additional calculations, performed directly by the Safety Assessment team are added. After presenting all these results, there is an evaluation of the degree to which the criteria and additional considerations are fulfilled with respect to safety and what feedback may be given to the further Site Investigation and Repository Design work.

3.2 Geological features of relevance to safety

Geology provides the overall framework for the other geoscientific disciplines and is consequently indirectly of fundamental importance for safety. Furthermore, some geological characteristics, i.e. the rock types, the deformation zones and the fracturing, are of direct relevance for safety. These are assessed in this section.

3.2.1 Criteria and other safety considerations

Previously set criteria

The suitability criteria, as set out by SKB in /Andersson et al. 2000/, directly related to the geological description of the site, concern rock type distribution, deformation zones and fractures.

In order to mitigate the risk of future human intrusion it is set as a *requirement* that the rock types in the deposition area do not have ore potential and do not contain such valuable minerals as to justify mining at a depth of hundreds of metres. There is a preference for common rock types with no occurrence of valuable utility stone or industrial minerals. For the feasibility studies, this called for avoiding areas with known ore potential and heterogeneous or unusual bedrock. Furthermore, it was stipulated that if extensive occurrence of ore-bearing minerals is encountered during the Site Investigation the site should be abandoned.

Deformation zones are important to safety since they potentially could be re-activated, thus threatening the mechanical stability of the repository system. Usually they also have much higher hydraulic conductivity than surrounding rock mass. Depending on their mode of formation, deformation zones could be ductile or brittle. Many ductile zones are in fact quite tight hydraulically, but some ductile zones could have been re-activated in periods of brittle deformation.

It is *required* that regional[1] ductile deformation zones are avoided, if it cannot be shown that the properties of the zone do not deviate from those of the rest of the rock. There may, however, be tectonic lenses near regional ductile deformation zones that can be suitable for a deep repository. It is also required that deposition tunnels and holes may not pass through or be located near regional and local major brittle deformation zones and that deposition holes may not intersect identified local minor fracture zones. Moderate densities (fracture surface area per unit volume) of fractures and of deformation zones shorter than 1 km are preferable.

As a criterion for the Site Investigation, it is stated that if the repository cannot be positioned in a reasonable manner (would have to be split up into a very large number of parts) in relation to the regional and local major deformation zones, the site is not suitable for a deep repository. However, at the time of publishing the suitability criteria document no specific respect distances were defined. These have now been developed, see below.

Additional considerations

Since the issue of the SKB suitability criteria, there has been further evaluation /Munier and Hökmark, 2004/ of the potential for shear movement and what would be necessary respect distances. The findings are also reported in the SR-Can Interim report (see /SKB, 2004b/, Chapter 10). The findings are preliminary in the sense that they may be overly restrictive.

/Munier and Hökmark, 2004/ have reported a number of simulations of secondary faulting induced by earthquakes, using different models. In particular, the simulations addressed the following question: "If a deformation zone near or within the repository reactivates seismically, how far from the source fault is the secondary slip on target fractures within the limits of the canister failure criterion?" One aspect of the work is that it can be used to assess whether it is possible to avoid faulting exceeding a 0.1 m displacement across deposition holes by applying a "respect distance" with the following definition:

The respect distance is the perpendicular distance from a deformation zone that defines the volume within which deposition of canisters is prohibited, due to potential future seismic effects on canister integrity.

The results of /Munier and Hökmark, 2004/ have been used to define respect distances to be used in repository engineering and design. These are based on the condition that shear movements at the deposition holes larger than 0.1 m could impair the integrity of the copper canister. Table 3-2 shows a summary of their findings and should be read as follows: For each zone of a particular size, the width of the transition zone and the seismic influence distance are calculated. The respect distance is the larger of the two.

Table 3-2 implies that respect distances only need to be applied to deformation zones larger than 3 km. Based on the table Repository Engineering applies a minimum respect distance of 100 m to deformation zones larger than 3 km. Furthermore, in order to estimate the size needed for the repository, an assessment is made on how many potential deposition holes would need to be abandoned if a rejection criteria was applied to deposition holes intersecting too large fractures, as further discussed in section 3.2.6.

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[1] The expression "regional" zones concern zones longer that 10 km, "local major zones" concern zones in the length interval 1 to 10 km and "local minor zones" concern zones in the length interval 10 m to 1 km, see /Andersson et al. 2000/.

Table 3-2. Seismic influence distance and Transition Zone half width in relation to zone length using various assumptions. The respect distance is the larger of the transition zone half width and the seismic influence distance. (From /Munier and Hökmark, 2004/).

Zone size	Seismic influence distance estimated from dynamic analyses of source to target interaction (calculated induced displacement should be < 0.1 m)		Transition zone half width estimates	
	If > 100 m radius fractures avoided	If > 50 m radius fractures avoided	W/L ratio 2%	W/L ratio 1%
< 3 km	–	–	0 m – 30 m	0 m – 15 m
3 km – 10 km	200 m	100 m	30 m – 100 m	15 m – 50 m
> 10 km	200 m	100 m	> 100 m	> 50 m

The information in the table could also be used to estimate the potential for shearing of deposition holes in a Safety Assessment. If the respect distance is set to a minimum of 100 m, only deposition holes intersecting fractures of a radius larger than 50 m would have any possibility of hosting a shear movement exceeding 0.1 m, but as further discussed by /Hedin, 2005/ the maximum induced slip would only occur along minor portions of the reactivated fracture plane. The amount of deposition holes with such intersections can be estimated from the discrete fracture network model as further discussed in section 3.2.6. It should also be noted that the amount of affected deposition holes will, for several reasons, be much less than this amount.

Most, if not all, deposition holes intersected by unfavorable fractures will be identified, and would thus not be used for deposition. Additionally, only few of the potentially problematic fractures will host slip exceeding the canister failure criteria. Finally, the probability of an earthquake, sufficiently large as to trigger significant reactivation on fractures nearby, is less then one. These latter factors will be assessed in SR-Can, but not in the PSE.

3.2.2 Rock type distribution

According to SDM S1.2 three principal lithological domains have been defined in the subarea, an A domain that is dominated by the Ävrö granite and which dominates on the island of Ävrö, Hålö and the northern parts of the peninsula, B domains that is dominated by the fine-grained dioritoid (B), one of which dominates the peninsula, a C domain that is characterised by a mixture of of Ävrö granite and quartz monzodiorite on the cape of the peninsula, A fourth domain is made up a few scattered E domains of diorite to gabbro. According to the model, only domains A01, B01, and C01, indicated in see Figure 3-1, are present at depth within the Simpevarp subarea.

The mineral compositions of the rock domains are provided in Tables 11-1 to 11-3 in SDM S1.2, and summarised in Table 3-3 below.

According to SDM S1.2, the confidence of occurrence and geometry of the rock domains at the surface is judged to be medium to high in the part of the local scale model area that is covered by the bedrock map of the Simpevarp subarea, and low to medium outside the Simpevarp subarea. Uncertainty in the three-dimensional geometry of the rock domains inside the Simpevarp subarea is caused by the still rather limited subsurface information and the fact that the overall geology is a pristine igneous bedrock terrain with little structural control. However, the rock type variation is within the bounds of the three rock domains, summarised in Table 3-3.

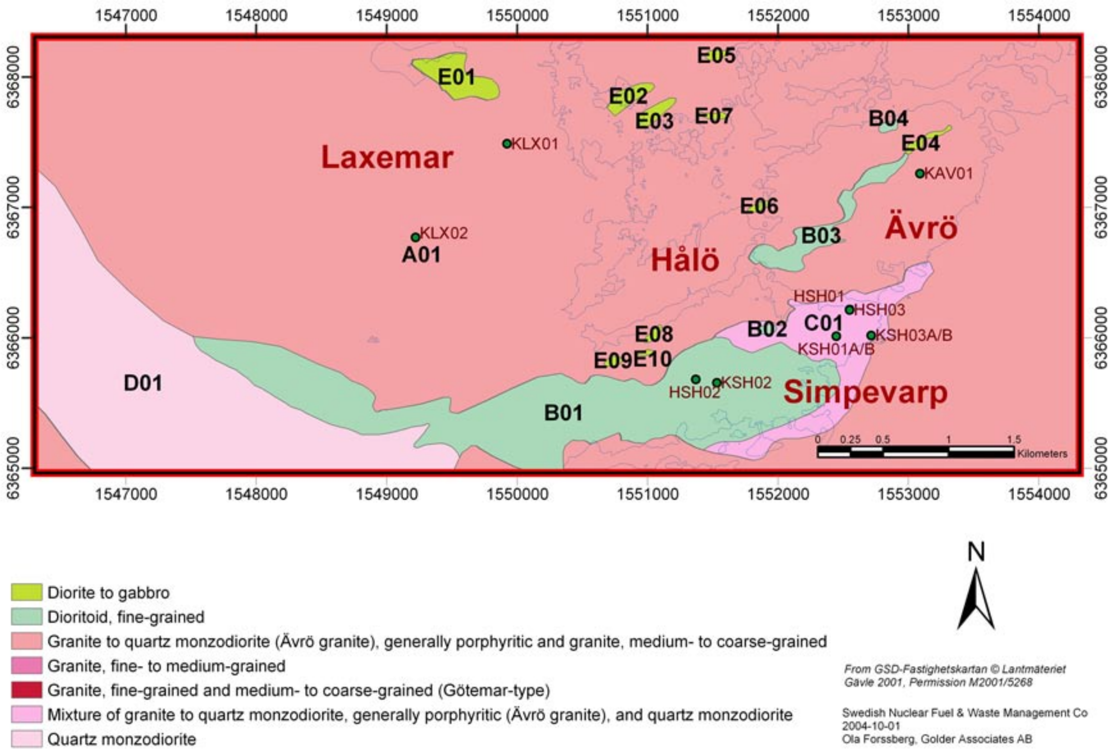

***Figure 3-1.** Surface view of the rock domains in the model. Only domains A01, B01, B02 and C01 are present at depth within the Simpevarp subarea (Figure 5-43 of SDM S1.2).*

Table 3-3. Composition of the rock domains in the Simpevarp Subarea (compiled from Tables 11-1 to 11-3 in SDM S1.2).

Rock domain	Main rock type(s)	Subordinate rock type
RSMA01 (Ävrö granite)	Ävrö granite: 75.8–84%	Fine- to medium-grained granite: 0.8–21.5%, Pegmatite: –, Fine-grained dioritoid: 9.0–17.0%, Diorite to gabbro: 0–1.7%, Fine-grained mafic rock: 3.0–4.9%, Quartz monzodiorite: –
RSMB01 (fine-grained dioritoid)	Fine-grained dioritoid: 90.6–94.2%	Quartz monzodiorite: 0–3.5%, Fine-to medium-grained granite: 0.9–6.7%, Pegmatite: 0.8–1%, Fine-grained mafic rock: 0.6–0.8%
RSMC01 (mixture of Ävrö granite and quartz monzodiorite)	Quartz monzodiorite: 51.5–73.9% Ävrö granite: 22.9–34.1%	Fine-grained dioritoid: 6.5%, Fine- to medium-grained granite: 1.8–4.2%, Granite: 2.0%, Fine-grained mafic rock: 1.2%, Pegmatite: 0.3–1.4%, Diorite to gabbro: 0.2%

3.2.3 Assessment of ore-potential

The ore potential of the site has been assessed by an ore exploration company (/Lindroos, 2004/, see also section 5.3.4 of SDM 1.2). In that work, ore potential was defined as mineralisations considered worthwhile to explore today or over a longer period. It is concluded that the Simpevarp regional model area is dominated by intrusive rocks and granites, belonging to the c. 1,810–1,760 Ma generation of the Transscandinavian Igneous Belt (TIB), which by experience is more or less devoid of metallic mineralisation. The only candidate for metallic mineralisation in the Simpevarp regional model area is the c. 1,450 Ma old Götemar-type granite, which is judged to have a potential for tin (Sn) and tungsten (W), although no mineralisations of this type have so far been found.

Consequently, the whole Simpevarp regional model area may be considered as sterile concerning metallic mineralisations and ores. Furthermore, the only real potential for quarrying building- and ornamental stone is associated with the Götemar and Uthammar granite intrusions in the north and south, respectively, i.e. well outside the Simpevarp subarea.

3.2.4 Deformation zones and fractures

Deterministic deformation zones

In the Site Description, the deformation zone model is developed for the entire regional domain of the Simpevarp area. A total of 188 deformation zones are identified but, of these, only 22 are judged to be of "high confidence", whereas the remaining 166 are labelled as "possible", see Figure 3-2. The confidence rating concerns the existence of the zone.

The twenty-two "high confidence" deformation zones are based, at least in part, on geological and geophysical data, such as borehole intercepts or clear surface expressions, supporting that these deformation zones do in fact exist. The support for the "possible" zones is weaker, as they are essentially only based on the outcome of a linked lineament interpretation, i.e. by assessing topographical and (airborne) surface geophysical data. Smaller zones and fractures, with a surface extent of less than 1 km, have not been included deterministically in the model, but are handled in a statistical way through discrete fracture network (DFN) models.

It is also stated, see section 5.4 of SDM S1.2, that there remains a clear possibility that one or more additional deformation zones will be recognised/interpreted in later modelling phases, following completion of more surface and borehole investigations in the Simpevarp and Laxemar subareas. The presented Simpevarp 1.2 model of deformation zones consists of only one "base case" model. Alternative models for deformation zones have not yet been developed.

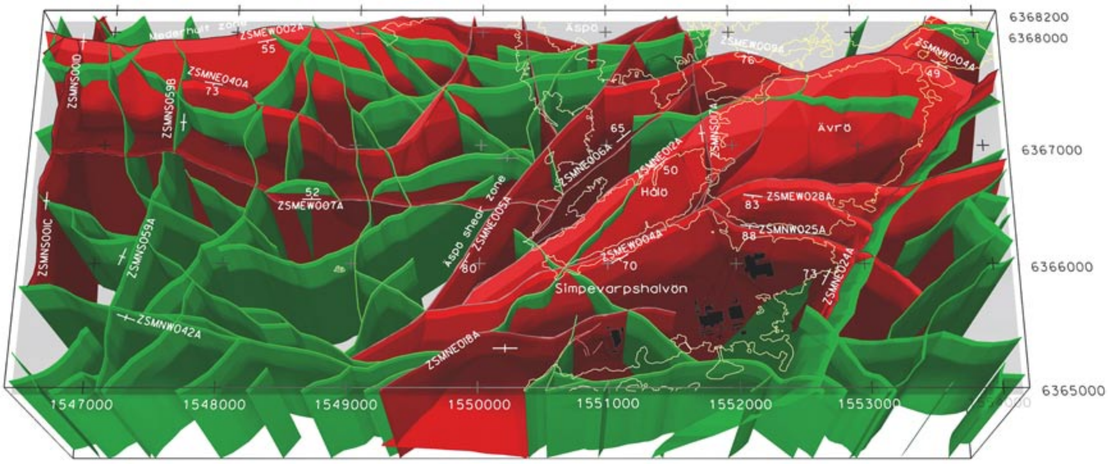

Figure 3-2. *Simepvarp 1.2 local model domain with interpreted high confidence and possible deformation zone. High confidence zones are indicated in red, possible zones in green (Figure 11-8 in SDM S.1.2).*

Also on the local model domain most interpreted deformation zones are classified as "possible", but the confidence is higher within the Simpevarp subarea. There, most of the zones in the model are considered to be of "high confidence" and only few are classified as "possible", see Figure 3-2.

Apart from the varying confidence in the existence of the zones there is also uncertainty in the continuity along strike and at depth, dip and termination; and in the character and properties (i.e. width, internal structure, fracturing, hydraulic properties) and spatial variability along zones. Quantified estimates of these uncertainties are given in the SDM S1.2. These uncertainties also apply to the high confidence zones. However, it should be noted also that these uncertainties are less inside the Simpevarp subarea than in the overall local domain.

The model description of the deformation zones contains information on observed ductile and brittle deformation. Some of the zones in Figure 3-2 are clearly only ductile, with little impact on permeability or potential for future reactivation and this of possibly little concern for safety or engineering. However, other ductile deformation zones show signs of later brittle reactivation. From a safety point of view all modelled deformation zones thus needs to be considered, at least until their characteristics are further established.

Statistical discrete fracture network model

Smaller zones and fractures, with a surface extent of less than 1 km, are handled in a statistical way through DFN models. The descriptions are based on fracture observations in the boreholes, mapped fractures on outcrops and from interpretation of lineaments. Several assumptions are needed when constructing these models, see section 5.5.1 of SDM S1.2. Therefore, two alternative models are presented in SDM S1.2. Model 1 relates three of the near-vertical orientation sets to three lineament sets, whereas the other near-vertical sets are unrelated to the lineament sets. In Model 2, all six near-vertical sets are related to lineament sets. Both models also have a subhorizontal orientation set. In addition, the DFN-model was modified by the hydrogeogological modelling teams to better fit the observed intensity of subhorizontal fractures in the boreholes, resulting in yet another alternative DFN-model, the Hydro-DFN model.

The corresponding DFN parameters for "Model 1" and "Model 2" are compiled in Tables 11-5 and 11-6 of SDM S1.2. The DFN model parameters used by the hydro-geological teams are provided in Tables 8-16 and 8-17 of SDM S1.2.

The variety of alternative DFN-models demonstrates that there are several uncertainties in the DFN-modelling. Of particular concern is the uncertainty in the fracture intensity for fractures sizes ranging from 10 to a 1,000 m scale and the uncertainty in the spatial variation of the fracturing, see SDM S1.2 for further details. The uncertainties are only partially quantified, although the different alternatives provide an indication of the uncertainty. Specifically, it is noted that the sub-horizontal fractures are estimated partly on surface data (size) and partly on borehole data (orientation and intensity).

Verification tests show that simulated intensity of subhorizontal fractures, in both Model 1 and Model 2 are currently overestimated by about a factor of two compared with observations in boreholes. The main reason for this may be the poor definition of subhorizontal fracture orientation and the size estimation. Relatively small samples of subhorizontal traces from outcrop have been used for estimating size, and these traces are considered to be highly uncertain due to the low angle of intersection with the outcrops. Thus, decision to base the intensity estimate more on outcrop data, than on the borehole data affects this bias.

As noted above, since the subhorizontal fractures are judged essential for connectivity, yet another DFN-model, a Hydro-DFN model, was developed for use in the hydrogeological modelling. In this model, the intensity of subhorizontal fractures is fitted to match the observed intensity in the boreholes.

3.2.5 Layout adaptation to deformation zones

Deposition volumes

For deformation zones longer than 3 km, the layout D1 design work for the Simpevarp subarea /SKB, 2005b/ applies a respect distance equal to the zone width or at least 100 m, i.e. in accordance with the rules defined in Table 3-2. For shorter zones, a margin for construction is applied that equals the zone width plus a safety margin based on potential construction problems, i.e. the applied rule is somewhat stricter than the safety related respect distance as given by Table 3-2. Zones of lower confidence, the possible zones, do not have widths given in the SDM S1.2. For these zones, the width is set to one percent of the length plus an additional 5 m safety margin. Figure 3-3 shows resulting respect distances at the –500 m level and includes both the high confidence and the possible deformation zones. There is little difference in the available area at the –400 m level.

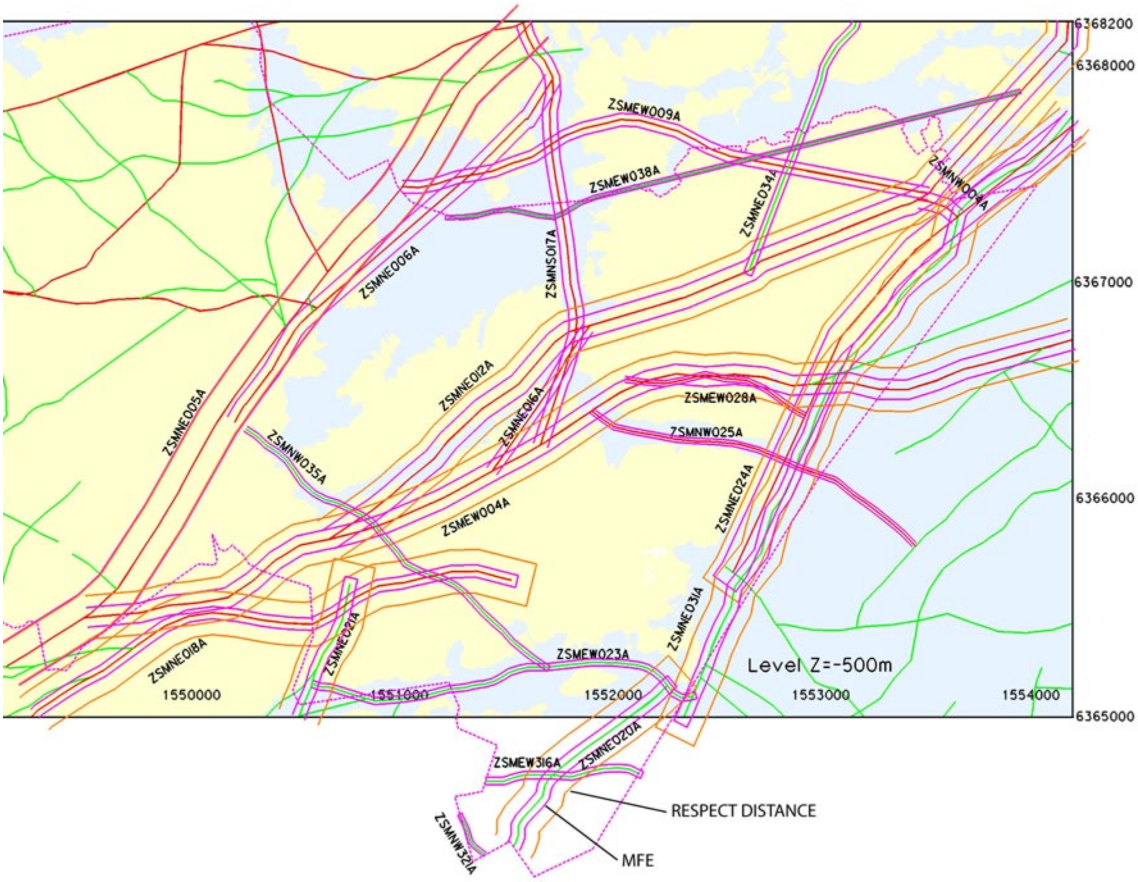

Figure 3-3. Respect distances and Margins for Constructions at the –500 m level considering both high confidence (red) and possible (green) deformation zones. (From /SKB, 2005b/).

The potential repository layouts presented for the Simpevarp subarea are based on the current Site Description. Later versions of the layout would of course need to incorporate any modifications of the Site Description, including changes of the deformation zone geometry.

The area of the rock actually needed for the repository depends on the number of canisters, the thermal properties and the "degree-of-utilisation". The latter depends on the mechanical stability, the probability of deposition holes intersecting fractures or deformation zones with radius R > 100 m, and the inflow of water to tunnels and deposition holes, see the design premises document /SKB, 2004c/. As already mentioned in section 2.2, the premises of the design work were for 4,500 canisters plus space for an additional 1,500 canisters. Using this information, the modelled thermal properties and the assessment of degree of utilisation the layout D1 design work for the Simpevarp subarea /SKB, 2005b/ presents potential layouts adapted to the respect distances. Figure 3-4 shows a potential layout at the –500 m level. Layouts at the –400 m level are also developed and they need about the same area. If only the high confidence zones are considered the required area is reduced by 12–13 percent and the number of deposition units is also reduced.

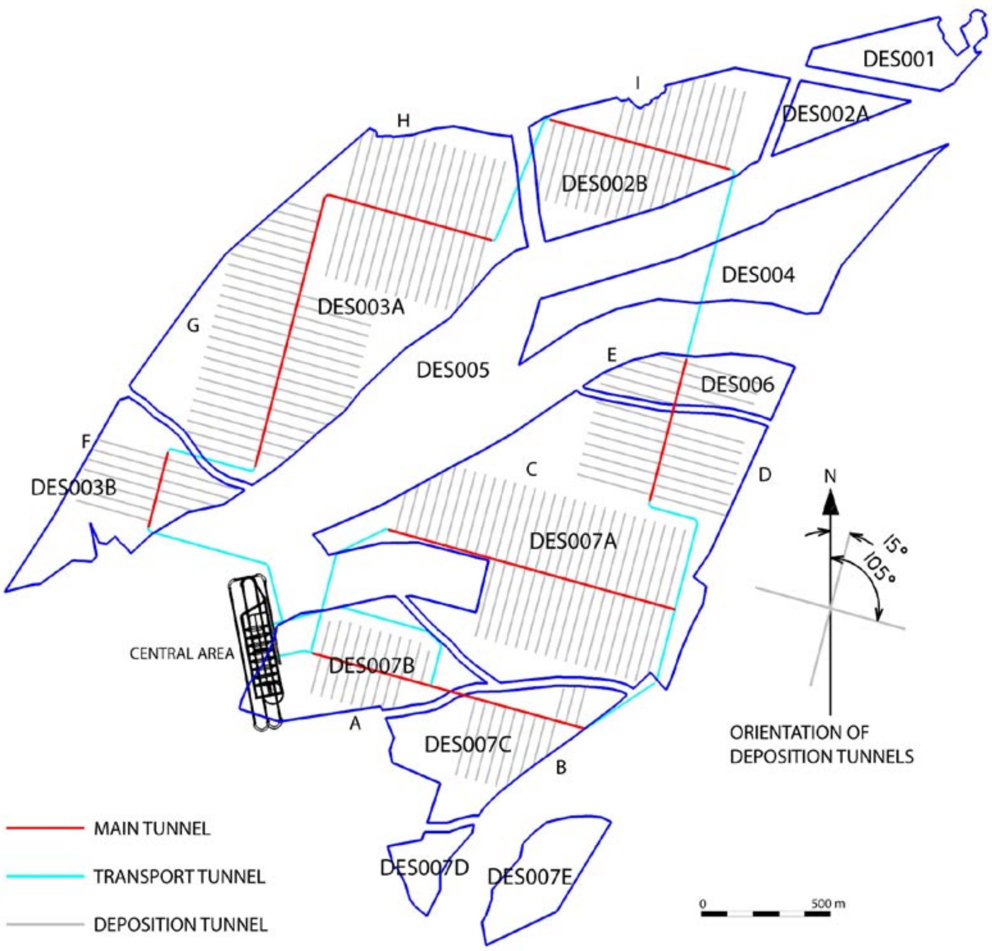

Figure 3-4. *Potential Layout at the –500 m level. (From /SKB, 2005b/).*

The layout D1 design work for the Simpevarp subarea /SKB, 2005b/ also presents a sensitivity study, exploring the effect of extending deformation zones ZSMNE018A and ZSMNE024A, changing the dip of zones 15° in the least advantageous direction for the layout, increased rock permeability by +5 percent, decreased rock permeability by –5 percent , decreasing the degree of utilisation by 2 percent and increased maximum length of deposition tunnels to 600 m. The analysis suggests that these rather drastic changes would, at most, require an increase in the deposition area by 5–6 percent.

In conclusion, the analysis suggest that there is sufficient space, with margin, for a repository within the Simpevarp subarea, taking into account respect distances to both high confidence and possible deformation zones, the assessed degree of utilisation and also considering the sensitivity to the site data. However, it should be noted that data on rock properties for the potential repository volumes at this time only exist from the Simpevarp peninsula and the Ävrö island. Hence, the suitability of rock volumes north of the deformation zone ZSMNE012A (DES001–DES003) is currently more uncertain than south of that zone.

3.2.6 Probability for deposition hole intersections with fractures and deformation zones

Degree of utilisation assessed by rock engineering

The fracturing of the rock affects the degree of utilisation, i.e. the number of potential deposition holes that would need to be discarded since they would be improperly located with respect to the fracturing of the rock. The main reason to discard a deposition hole would be if it intersected the central parts of a too large fracture, see section 3.2.1.

The procedure stipulated in the design premises /SKB, 2004c/ requires that the degree of utilisation is calculated by assuming that deposition holes are rejected according to a distance criterion stipulated as the smallest allowed distance between fractures or deformation zones and the perimeter of deposition holes:

- 2 m for fractures/zones in the interval $100 < R \leq 200$ m.
- $0.01 \times R$ for fractures/zones with $R > 200$ m.

This distance criterion deviates from the simpler rule stating that with 100 m respect distance, deposition holes must not be placed in the central parts of fractures with radius $R > 50$ m. The number of rejected deposition holes resulting from applying i) the engineering criterion or ii) this latter rule, is assessed in the next subsection.

In order to assess the consequence of the engineering criterion, simulations with the Discrete Fracture Network models, see section 3.2.4, have been carried out as a part of the layout D1 design work for the Simpevarp subarea /SKB, 2005b/. There fractures/features were simulated in a model box and then the distance between the simulated fractures and simulated deposition holes were calculated. If the deposition hole is closer than a certain distance, the location is rejected in the model. The simulations are carried out for a 300 m long tunnel with 20 realisations for each tunnel orientation. For each deposition hole, all fracture sizes within 2 m from the hole perimeter are recorded. In addition, all fractures less than 2 m below the floor of the holes are recorded. This technique may also be described as being equivalent to drilling a 10 m deep shaft with radius 2.875 m, instead of a deposition hole and recording all fractures within this volume. This is then repeated for each deposition hole, in each realisation. Hence, the criteria for rejection of deposition holes "0.01R for fractures/zones with $R > 200$ m" is not taken into account in this evaluation. The method is illustrated in Figure 3-5.

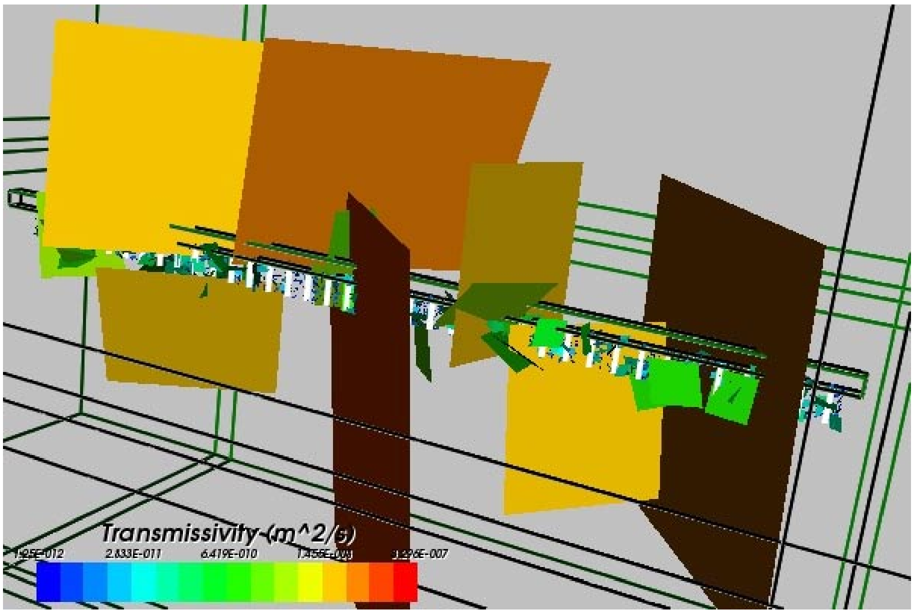

Figure 3-5. Tunnel with deposition holes represented by shafts. Only those fractures that are within 2 m of a shaft are shown, coloured by transmissivity. (From /SKB, 2005b/).

Applying this method with the Hydro-DFN model, the percentage of holes with fractures larger than R = 100 m closer than 2 m from a hole perimeter for different tunnel orientations is calculated to be on average about 10 percent, see /SKB, 2005b/.

Complementary evaluation

A much simpler method, than to carry out numerical simulations with a DFN-model, for calculating the probability of a canister location being intersected by a fracture exceeding a prescribed size[2] is presented in /Hedin, 2005/. The method is analytical and is based on the particular types of statistical descriptions of fracture sizes and orientations that emerge from the site investigations. Furthermore, the analysis is based on the full fracture population i.e. the DFN-parameters representing both "open" and "sealed" fractures.

Applying the analytical calculation to the case simulated within the design work, and using the Hydro-DFN model results in 13.4 percent rejected positions. This value is higher than the 10 percent obtained by the simulations made in the design study and reported above, since too small a model volume to house all potentially intersecting large fractures was used in that simulation. Independent simulations within the framework of the analytic model confirm that around 10 percent is obtained with the restricted model volume and that the theoretically calculated 13 percent is obtained with a sufficiently large simulation model volume.

The issue of large fractures intersecting deposition positions is however different from the perspectives of design and long-term safety. The design rule described above aims at excluding all deposition positions where detrimental shear movements could possibly occur. The observable indications of a sizeable fracture may occur over a finite distance from the plane of a potential shear movement, hence a rather extended volume around a deposition position is considered in the design rule. From the point of view of long-term safety, the

[2] Without considering the probability of detecting such fractures.

issue is to determine the risk of *canisters actually being intersected by discriminating fractures*. If it is pessimistically assumed that none of the discriminating fractures can be detected (i.e. if the design rule were ineffective) what is the likelihood that a randomly emplaced canister is intersected by a discriminating fracture? The calculation problem is the same as that for the design rule, but now applied to a volume equal to that of the canister, rather than to the extended deposition hole volume considered in the design calculation.

The calculated portion of *canisters* being intersected by discriminating fractures of radius larger than 100 m is about 2.8 percent and the calculated portion of canisters being intersected by discriminating fractures of radius larger than 50 m is 5.5 percent. These values are much less than the 13.4 percent resulting from the current design rule. The difference is due to the considerably smaller volume in the safety assessment calculation, as explained above, and also to the fact that the outermost part of a discriminating fracture is excluded from this calculation, since the movement in that part of the fracture is assumed too small to damage the canister, see further /Hedin, 2005/.

In order to assess the importance of the properties of the DFN-model, the portion of *canisters* being intersected by discriminating fractures of radius larger than 100 m is also calculated for the DFN model 2 suggested by geology, see section 3.2.4. The calculated values are 2.5, 5.7 and 3.6 percent, for the respective rock domains. These values are generally higher than the 100 m results of the Hydro-DFN-model, which appears reasonable since the geological model overestimates the fracture intensity in the rock. It should also be noted that in DFN-model 2, the size model for the sub-horizontal set is given as a log-normal distribution. This distribution is valid for fracture sizes up to a few standard deviations above the mean value of the distribution, i.e. for fracture radii up to roughly 10 m in this case, and cannot be used to estimate ε, which requires a distribution valid for fracture radii up to 500 m. For the conceptual DFN model 1, four of the seven fracture sets are given as log-normal distributions, and this model was therefore not used to estimate the portion of canisters being intersected by discriminating fractures. In fact, using a log-normal distribution for the sub-horizontal set appears quite unfounded, since there is no length data on this set. It would appear more natural to assume the same length distribution for the sub-horizontal set as for the vertical sets.

The results are very sensitive to variations in k, the exponent of the power-law distribution. The sensitivity to e.g. details of the orientation distribution of fractures is considerably less pronounced, see further /Hedin, 2005/. The sensitivity to *k* reflects the fact that the power-law size distributions cover a large span of fracture radii in the calculations. Observations are however essentially available on the metre to tens of metre scale and on the scale of 1,000 m and larger. Observations in the size interval that causes the discriminating fracture intersections in the calculations cited above, i.e. one to several hundred metres, are scarce. It is therefore desirable to increase the confidence in this interval of the size distributions.

3.2.7 Safety implications

The previous sections show that the Simpevarp subarea meets all geological requirements and preferences, although there are considerable uncertainties in the statistical fracture model (the DFN-model):

- It is well established that the Simpevarp subarea does not have any ore potential. The rock type distribution represents typical crystalline basement rock and the remaining uncertainties are of little concern for safety.

- It appears possible to locate a sufficiently large repository within the subarea, while meeting the required respect distances to the deformation zones. The layout presented for the –500 m level considers both high confidence zones and possible zones. If only high confidence zones are considered, the required repository area decreases by about 12 percent. Furthermore, the sensitivity analysis on how the available deposition area would change due to uncertainties in the geological model shows only a moderate impact on the space requirement. However, the confidence in the model north of zone ZSMNE012A is limited.
- Even if there are uncertainties in the DFN-models presented, the calculated portion of canisters being intersected by discriminating fractures of radius larger than 50 m is in the order of a few percent. This number of potentially unsuitable deposition holes is much less than what is considered in the layout when assessing the degree of utilisation. For the Safety Assessment, there is also a need to consider the probability of actually finding the deposition holes intersected by large fractures. Initial such assessments, focusing on finding how good such practical identification needs to be, in order to make the impact of post-glacial faults negligible, will be made in SR-Can.

Even though the geological requirements and preferences are already considered to be met, further reduction of the uncertainties in the structural and DFN geological model would enhance the safety case and would also allow for a more efficient design:

- Reducing the uncertainty on the deformation zone geometry, including reducing the amount of "possible" deformation zones in relation to the "high-confidence" ones, would allow for a better specified layout, and the additional data as suggested by SDM S1.2 and subsequent evaluation would be useful. Especially, data on deformation zones and rock properties for the potential deposition areas north of ZSMNE012A would reduce uncertainties in the degree of utilization for this part of the Simpevarp subarea.
- There is substantial uncertainty in the DFN-model. Various alternatives have been presented but it is not clear that these alternatives span the uncertainty space. Efforts need to be spent on reducing these uncertainties. During the Site Investigation Phase this can partly be achieved with more data, as further discussed in Chapters 12 and 13 of SDM S1.2, but there is a limit on the extent to which these uncertainties could be reduced using only surface based information. Efforts need also be spent on improving the modelling. There are assumptions made in current models that could be challenged and there seems to be room for better use of the borehole information. It is especially important to provide robust estimates of the intensity of large fractures and features, e.g. the *k* parameter in the power-law distribution and further efforts should be spent on providing good support for the possible range of this parameter. In contrast, details of the orientation distribution of fractures are of much less importance.

Finally, it is noted that the design rules for discarding canister positions due to potential intersections with too large fractures or deformation zones are overly restrictive. The percentage of deposition holes to be discarded would substantially decrease if the design rules were better harmonised with the actual safety requirements.

3.3 Rock mechanics

Many of the requirements and preferences relating to rock mechanics concern implications for Repository Engineering. However, there are also important safety considerations. Especially, it is important to understand the mechanical stability of the deposition holes.

3.3.1 Criteria and other safety considerations

Previously set criteria

The suitability criteria, as set out by SKB in /Andersson et al. 2000/, directly related to the rock mechanics of the site, concern initial rock stress and rock mechanics properties of the intact rock, the fractures and of the rock mass.

In order to ensure safe working conditions and that the deposition hole geometry will be within given tolerances, it is *required* that extensive spalling or other extensive overbreak may not occur within a large portion of the deposition area. The fulfilment of this requirement is to be verified by means of a site-specific analysis. There is *preference* for normal stress levels (and considerably lower than 70 MPa), and intact rock strength and deformation properties that are normal for Swedish bedrock.

It is further stated that the calculated stress situation in the rock nearest the tunnels and the resultant rock stability during and after the construction phase is used mainly to adapt repository depth and layout. If the repository cannot be reasonably configured in such a way that extensive and general stability problems can be avoided, the site is unsuitable and should be abandoned. Extensive problems with "core disking" should give rise to the suspicion that problems may be encountered with spalling during tunnelling. There should also be special attention given to the rock mechanics issues if the strength of the rocks deviates from normal values in Swedish bedrock.

There are no requirements on the rock mechanics properties of fractures and fracture zones or of the rock mass. It is noted that these properties are used by Repository Engineering for developing the layout and for making a constructability forecast. Good constructability is of course advantageous.

There is no requirement on the coefficient of thermal expansion, but it is discussed whether an inhomogeneous expansion could impair the stability of deposition holes. Therefore, there is a *preference* for normal values for Swedish bedrock and with limited inhomogeneity.

Additional considerations

There are no additional considerations. The possibility and consequences of spalling in deposition holes due to the thermal load are to be explored within SR-Can, see also Chapter 10 of SR-Can interim /SKB, 2004b/. It seems likely that inhomogeneity in thermal expansion itself would not be an issue. If there is a risk of thermally induced spalling, it would occur in the rock type with the lowest strength.

3.3.2 Stress and rock mechanics properties

In the SDM S1.2, the stress estimations are presented for two defined stress domains included in the local scale model area, see Figure 3-6. Most of the Simpevarp subarea is located in stress domain II, but there are also some parts in stress domain I. The estimated stress magnitudes are given in Table 3-4 and Table 3-5. As can be seen, stress levels are higher in domain I.

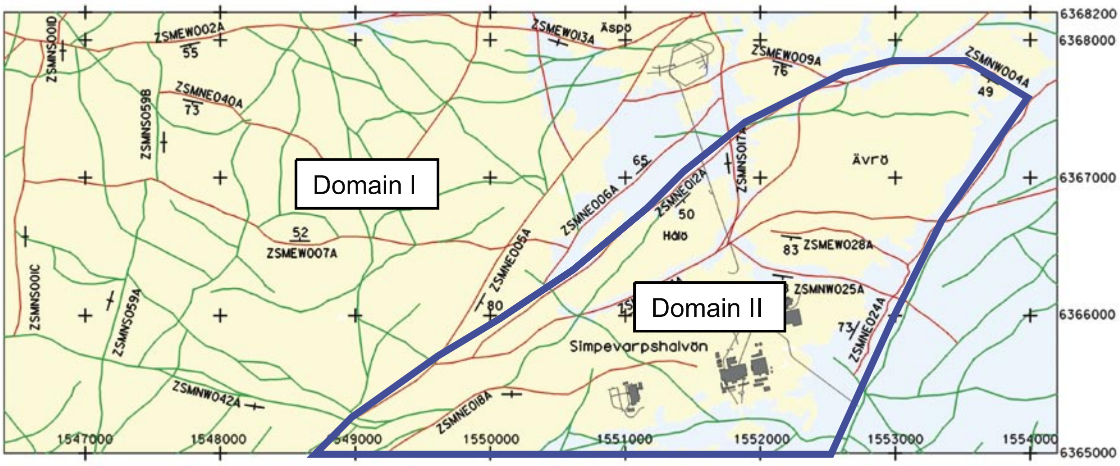

Figure 3-6. *Stress domains I and II in the stress model. Stress Domain I is NW of zone XSMNE012A (dipping SE) and SW of zone ZSMNW024A (dipping NW) and stress Domain II is located in the wedge-shaped domain between the zones (Figure 6-20 in SDM S1.2).*

Table 3-4. Model of *in situ* stress magnitudes in the Simpevarp 1.2 stress domain I (Table 6-8 in SDM S1.2).

Parameter	σ_1	σ_2	σ_3
Mean stress magnitude, z = depth below ground surface (m)	0.058·z+3 MPa	0.028·z MPa	0.019·z MPa
Uncertainty, 100–1,100 m	± 30%	± 30%	± 30%
Spatial variation in rock domain	± 15%	± 15%	± 15%
Spatial variation in or close to deformation zones	± 50%	± 50%	± 50%

Table 3-5. Model of *in situ* stress magnitudes in the Simpevarp 1.2 stress domain II (Table 6-10 in SDM S1.2).

Parameter	σ_1	σ_2	σ_3
Mean stress magnitude, z = depth below ground surface (m)	0.032·z MPa	0.018·z MPa	0.011·z MPa
Uncertainty, 100–1,100 m	40%	40%	40%
Spatial variation in rock domains	15%	15%	15%
Spatial variation in or close to deformation zones	50%	50%	50%

Uncertainties in rock stress magnitudes and distribution within the model area are due to data inaccuracies (see Chapter 12 of SDM S1.2) and limited information density. However, inside the Simpevarp Peninsula the understanding of the stress field is judged to be good. It should be noted that the division into two stress domains is based on available information up till now. For stress domain I, which covers the Laxemar subarea, this includes overcoring in only one borehole in the Laxemar subarea. This model of the Laxemar subarea may be changed at later stages of the site investigation, as new measurement data will become available, but would not significantly affect the stress modelling of stress domain II, where there is more data. The higher stresses in the northwest part of the Simpevarp subarea belonging to stress domain I are also quite certain as this part lies close to the Äspö HRL, where there are numerous stress data.

Rock mechanics properties of intact rock

The rock mechanics properties of the intact rock, together with the rock stress, affect the risk of spalling, both during construction and as a result of the thermal load. The estimated properties of different rock types in the area are provided in Table 3-6. The uncertainty ranges are judged to cover both uncertainty and spatial variability. Uncertainties in rock mechanical properties of Ävrö granite intact rock are due to lack of new laboratory tests. Old data from Äspö have been used, but there are uncertainties in the quality of these data. Furthermore, these data have a low spatial coverage, i.e. may give rise to bias. However, this uncertainty is judged to only have a minor effect on the assessed rock mass properties.

Rock mechanics properties of the rock mass

The rock mechanics model also covers properties of the rock mass. These properties are important for Rock Engineering, but have few direct safety implications. Therefore, these properties are not summarised here.

Coefficient of thermal expansion

As further explained in section 7.2.6 of SDM S1.2 the coefficient of thermal expansion was measured on samples from three different boreholes; KAV01, KSH01A and KSH02 in the Simpevarp subarea /Åkesson, 2004a,b,c/. The coefficient is found to vary between $(6.0–8.0)\times10^{-6}$ K^{-1} for the three dominating rock types.

Table 3-6. Estimated rock mechanical properties for intact rock (matrix) of the dominant rock types (i.e. small pieces of rock without any fractures). The truncation values are not necessarily symmetrical with respect to the mean as they are selected not only based on the observed data but also on expert judgement (Table 6-5 of SDM S1.2).

Parameter for intact rock (drill core scale)	Quartz-monzonite to monzodiorite and Ävrö granite		Finegrained dioritoid	
	Truncated normal distribution Mean/standard dev.	Min (trunc.) – Max (trunc.)	Truncated normal distribution Mean/standard dev.	Min (trunc.) – Max (trunc.)
Uniaxial compressive strength, UCS	165 MPa / 30 MPa	110 – 200 MPa	210 MPa / 50 MPa	120 – 265 MPa
Crack initiation stress, σ_{ci}	0.47 × UCS	0.47 × UCS	0.47 × UCS	0.47 × UCS
Young's modulus	80 GPa / 10 GPa	70 – 90 GPa	85 GPa / 10 GPa	70 – 110 GPa
Poisson's ratio	0.27 / 0.05	0.18 – 0.33	0.26 / 0.03	0.19 – 0.31
Tensile strength	17 MPa / 4 MPa	12 – 24 MPa	20 MPa / 2 Mpa	14 – 24 MPa
Mohr – Coulomb, F*	60° / 3°	57° – 62°	55° / 6°	35° – 60°
Mohr – Coulomb, c*	22 MPa / 3.2 MPa	14 – 29 MPa	32.5 MPa / 5.4 MPa	20 – 42 MPa

* The cohesion and the friction angle are correlated with correlation coefficients of –0.327 for Quartz monzonite and –.2413 for Finegrained dioritoid (higher friction angle is correlated with lower apparent cohesion).

3.3.3 Mechanical stability during construction and operation

The layout D1 design work for the Simpevarp subarea /SKB, 2005b/ (also published as /Martin, 2005/) assessed the risk of spalling of deposition tunnels and deposition holes, using the stress and intact rock properties discussed in section 3.3.2. The following conclusions, see also Figure 3-7, are made:

- In stress domain I there is a risk for spalling in the vertical deposition holes below a repository depth of 450 m. At 550 m the probability of spalling is approximately 20 percent, i.e. 20 percent of the deposition holes may be affected, whereas at a repository depth of 650 m the probability for spalling increases to approximately 70 percent. At a depth of 550 m the probability of spalling for these tunnels is approximately 10 percent. The risk for spalling in the deposition tunnels is eliminated if the deposition tunnels are oriented parallel to or at an angle less than 45 degrees to the maximum horizontal stress, regardless of the repository depth.
- In stress domain II, there is no potential for spalling in either the vertical deposition boreholes or the deposition tunnels, regardless of tunnel orientation relative to the maximum horizontal stress.

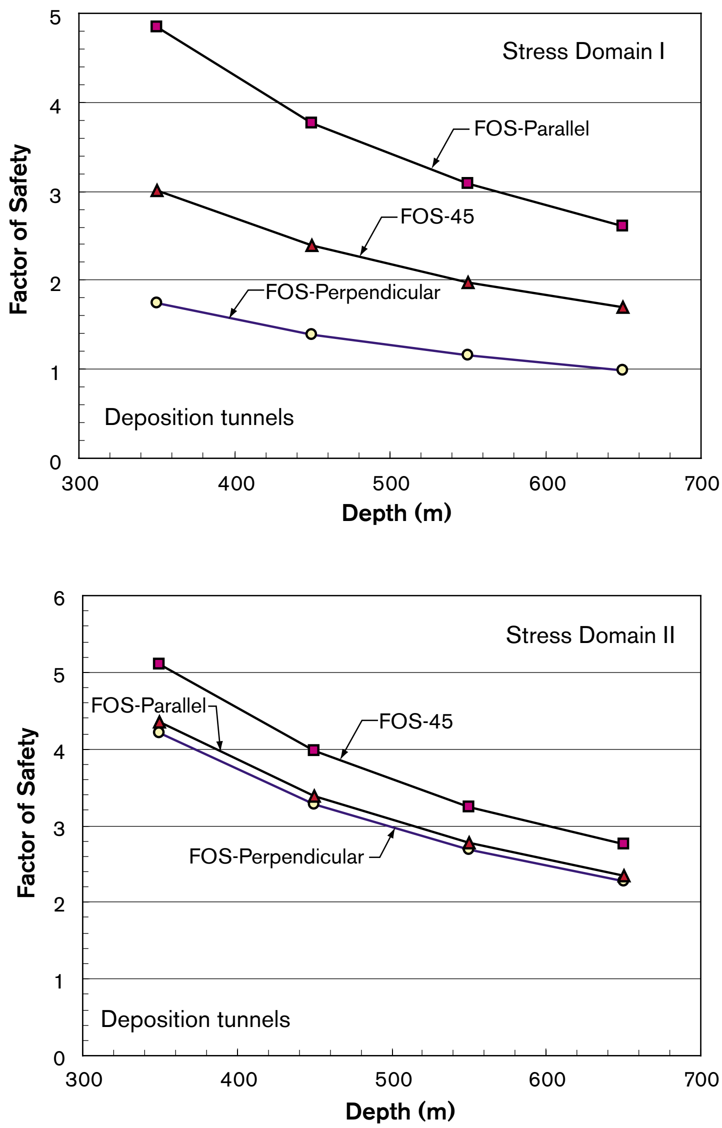

Figure 3-7. Spalling instability for deposition tunnels for Stress Domains I and II of Simpevarp. (From /Martin, 2005/).

The layout D1 design work for the Simpevarp subarea /SKB, 2005b/ suggests deposition tunnel directions that would avoid any spalling problems of the deposition tunnels.

3.3.4 Safety implications

The previous sections show that the Simpevarp subarea meets all the rock mechanics requirements and preferences:

- The rock mechanics properties of the intact rock and the *in situ* stress lie within ranges typical of Fennoscandian crystalline rock.
- In stress domain I there is a risk for spalling in the vertical deposition holes below a repository depth of 450 m and the risk increases with depth. The risk for spalling in the deposition tunnels is eliminated if the deposition tunnels are oriented parallel to or at an angle less than 45 degrees to the maximum horizontal stress, regardless of repository depth. In stress domain II, there is no potential for spalling in either the vertical deposition boreholes or the deposition tunnels, regardless of tunnel orientation relative to the maximum horizontal stress.
- There is only moderate variation in the coefficient of thermal expansion. The possibility and consequence of spalling in deposition holes due to the thermal load is an issue to be explored within SR-Can. However, such spalling is judged unlikely at the Simpevarp subarea due to the low stress levels.

Overall, it is considered that the current uncertainty in stress and intact rock properties is sufficiently low for making the safety case. However, the issue of spalling due to the thermal load may require additional analyses, as already envisaged for SR-Can. This may also lead to additional data demands.

3.4 Thermal analyses

The thermal conductivity of the rock mass affects the thermal evolution of the canister and the bentonite buffer. This is of importance for safety, since elevated temperatures on the canister and in the buffer may affect the properties of these important barriers. However, the temperature level could generally be controlled by an appropriate design.

3.4.1 Criteria and other safety considerations

Previously set criteria

The suitability criteria, as set out by SKB in /Andersson et al. 2000/, directly related to the thermal properties of the site concern the thermal conductivity and the initial temperature profile. The criteria are based on the *requirement* that the temperature on the canister surface and in the buffer must not exceed 100°C, in order to ensure predictable canister corrosion and buffer stability.

No requirements are set on the rock thermal conductivity, but a *preference* for thermal conductivity, which influences repository layout and repository size, larger than 2.5 W/(m·K) was given. It was also noted that, during the site investigation, detailed knowledge of rock types and thermal conductivity is used to adapt the repository layout.

Also, there are no requirements on initial temperature, although areas with potential for geothermal energy extraction (very high geothermal gradient) should be avoided. A *preference* was set that the initial temperature at repository depth should be less than 25°C.

Additional considerations

The premises for temperature restrictions on the canister surface are essentially still valid, as discussed in Chapter 6 of SR Can Interim Report /SKB, 2004b/. There, it is stated that the temperature at the canister surface should be restricted so that at the time when water comes in contact with the canister, boiling will not occur. Boiling may result in salt deposits on the canister surface and such deposits could cause corrosion in a way that is difficult to analyse quantitatively. Therefore, the temperature at the canister surface at water contact should be less than 100°C. This is essentially achieved by limiting the initial activity of the fuel in each canister and by adapting the layout of the repository.

No credit is taken for the effect of increased hydrostatic pressure on the boiling point, since it can not be guaranteed that this has developed when the peak temperature occurs. Nor is any credit taken for an increased boiling point due to solutes in the contacting water, since no minimum solute concentration can be guaranteed. The impact of the increase in air pressure, due to the low elevation in the repository, is also pessimistically neglected.

Also, the buffer temperature should not exceed 100°C in order to limit chemical alterations /SKB, 2004b/. The peak buffer temperature will, however, always be lower than the peak canister temperature, so that this criterion is automatically fulfilled if the criterion on canister surface temperature is fulfilled, with the possible exception of canister surface temperatures exceeding 100°C prior to water contact.

3.4.2 Thermal properties and initial temperature

Thermal conductivity and heat capacity

As further explained in Chapter 7 of SDM S1.2 the thermal conductivity at canister scale is modelled for the lithological domains of the Simpevarp subarea, using different modelling approaches. Results indicate that the mean thermal conductivity is expected to exhibit only a small variation between the different rock domains, from 2.74 W/(m·K) to 2.80 W/(m·K), see Table 3-7. The standard deviation varies according to the scale considered, and for the canister scale it is expected to range from 0.20 to 0.28 W/(m·K). The lower confidence limit, taking account of the spatial variation at the canister scale, is within the range 2.27–2.35 W/(m·K) for all four domains. The temperature dependence is rather small with a decrease in thermal conductivity of 1.1–3.4 percent per 100°C increase in temperature for the dominant rock types.

Table 3-7. Mean value, standard deviation and two-sided 99 percent confidence intervals of thermal conductivity (W/(m·K)) in each domain at canister scale. (Table 7-11 in SDM S1.2).

Domain	Mean	St. dev.	Lower confidence limit	Upper confidence limit
RSMA01	2.80	0.28	2.25	3.35
RSMB01	2.74	0.20	2.35	3.13
RSMC01	2.74	0.24	2.27	3.21

There is less variation in heat capacity with mean values ranging between 2.23 and 2.24 MJ/(m³·K) for the different rock domains, see Table 7-13 of SDM S1.2. The standard deviation small and is estimated to be about 0.1 MJ/(m³·K).

There are a number of important uncertainties associated with these results. One of the uncertainties relates to the representative scale for the canister. Another important source of uncertainty is the methodological issues associated with the upscaling of thermal conductivity from cm-scale to canister scale. In addition, the representativeness of rock samples is uncertain, with a possibility that some bias has been introduced by judgmental sample selection. Nevertheless, the uncertainty of thermal conductivity has been quantified as ranges, for different scales, although better understanding of the upscaling could possibly allow further variance reduction at the larger scales.

Initial temperature

As further explained in Chapter 7 of SDM S1.2 the *in situ* temperature has been measured in six boreholes. The temperature has been logged at different occasions in wo of them. The mean of all temperature loggings is 14.4°C at 500 m depth, see Table 7-8 of SDM 1.2.

Different loggings in the same borehole give slightly different results, indicating that there is a potential error. Possible sources of uncertainty in the temperature logging results include the timing of the logging after drilling, water movements along the boreholes, and errors in the measured inclination of the boreholes. The uncertainty is quantified as a range. It is small in absolute terms, but still potentially important for engineering and layout.

3.4.3 Thermal evolution of canister surface, buffer and near field rock for present climate conditions

Temperature calculations performed by rock engineering

In the layout work /SKB, 2005b/, the thermal properties and the initial temperature of the different rock domains are used to calculate the necessary distance between deposition holes, in order to ensure that the temperature criteria for the canister and the buffer are met. The design rule is provided in the Underground Design Premises document /SKB, 2004c/. The rule is based on the analyses performed by /Hökmark and Fälth, 2003/.

Table 3-8 shows the resulting minimum spacing for different depths and rock domains. The designed minimum canister spacing is based on the mean values of the thermal conductivity, 40 m separation between deposition tunnels and a heat capacity of 2.08 MJ/(m³·K), i.e. the heat capacity is cautiously chosen to be at the bottom of the observed range. In order to account for the spatial variability of the thermal conductivity, the design formula considers a safety margin of 10°C. Another 10°C safety margin is introduced to account for the gap between canister and buffer and the gap between buffer and rock. This means that the calculated peak canister temperature, before added safety margins, with the selected canisters spacing and for the mean thermal conductivity is about 80°C.

Table 3-8. Minimum required distance between deposition holes for different depths and for the mean value of thermal conductivity in the different rock domains. (From /SKB, 2005b/).

Depth (m)	*In situ* temperature °C	Minimum required distance between canisters (m)		
		Domain A: Ävrö granite (λ = 2.80)	Domain B: Fine grained dioritoide (λ = 2.74)	Domain C: Mixture of quartz monzodiorite and Ävrö granite (λ = 2.74)
400	13.2	7.1	7.3	7.3
500	14.8	7.3	7.5	7.5
600	16.3	7.8	8.1	8.1
700	17.6	8.4	8.7	8.7

Complementary temperature calculations

The safety margin used in the design work should account for most of the spatial variability of the thermal conductivity. However, in order to assess whether there is any likelihood of individual canisters reaching temperatures above 100°C, some additional calculations based on the thermal properties of the Simpevarp subarea are presented below. The analysis is otherwise based on the same premises as described in the SR-Can Interim report /SKB, 2004b/.

The peak temperatures as a function of time in the fuel, the cast iron insert, the copper canister, the buffer and the host rock are calculated using an analytic model /Hedin, 2004/. The model is based on analytical solutions describing the canisters as a set of point sources in the host rock and steady-state heat conduction expressions are used for heat conduction in the buffer. Furthermore, heat transfer due to combined radiation and conduction in the gaps between canister and buffer and in the canister interior are calculated analytically. That is, the analysis does not apply the added margins applied in the design work, it models the temperature drop over the canister/buffer and buffer/rock interfaces directly.

Similar treatments are presented for the host rock and buffer in /Hökmark and Fälth, 2003/. Benchmarking against the results of /Hökmark and Fälth, 2003/ and of numerical finite element calculations for buffer and rock yields discrepancies of peak canister peak temperatures of less than one degree /Hedin, 2004/.

Figure 3-8 shows the results of the complementary thermal calculation as the thermal evolution at a number of points located on a radius extending horizontally from the canister mid-point along the deposition tunnel. The peak canister surface temperature at the canister mid-height is 96°C, with data as listed in Table 3-9. The temperature decreases towards the end of the canister. When the peak canister temperature occurs, the temperature drop across the 5 mm gap between canister and buffer is 11°C meaning that the buffer inner temperature is 85°C. The corresponding drop across the 30 mm gap between buffer and rock wall is 6°C, from 64 to 58°C. Thus, of the 20°C safety margin applied by engineering only 4 is left for absorbing uncertainty and spatial variability of the rock thermal conductivity. This independent calculation implies that the inner buffer temperature would be 79°C disregarding the temperature drop across the outer gap, in close agreement with the 80°C target temperature employed in the design work where gaps are not taken into account.

It was cautiously assumed that no groundwater is taken up by the buffer, since this would lead to an increased thermal conductivity and eventually to a closure of the gaps at the buffer interfaces. The treatment also neglects the presence of the tunnel backfill above the deposition hole, but this has been demonstrated to influence the critical temperature only marginally /Hökmark and Fälth, 2003/.

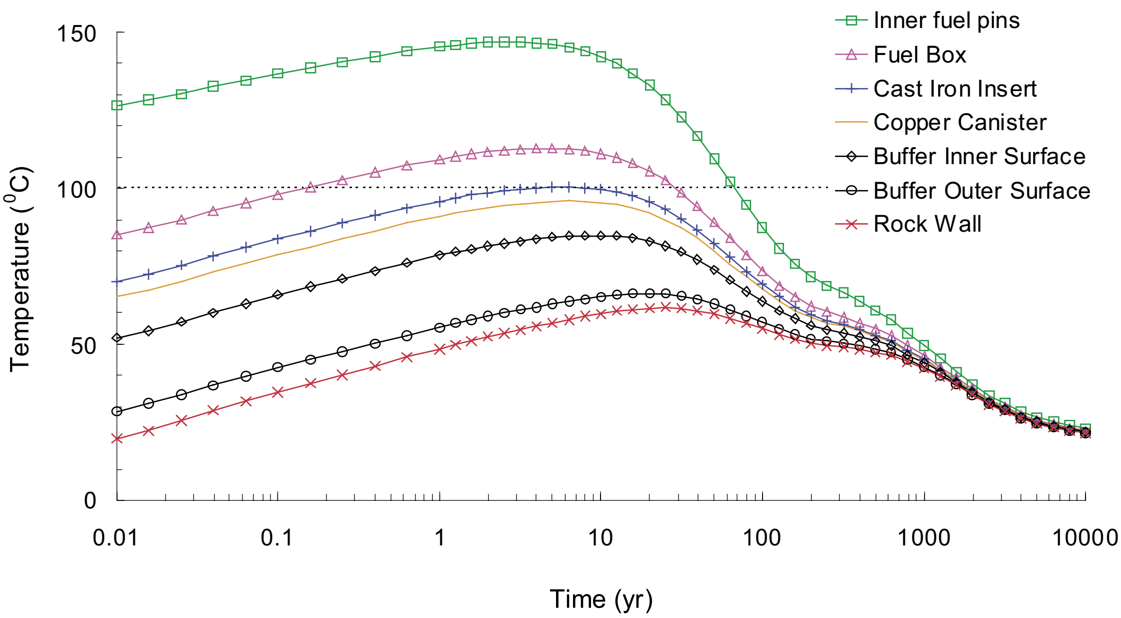

Figure 3-8. *The thermal evolution for a number of points at canister mid-height for data given in Table 3-9.*

Table 3-9. Thermal sub-model data for the central case presented in Figure 3-8. Site-specific data are taken from /SKB, 2005b/. The canister is assumed to be filled with air. All other data required for the calculation are given in Table 7-3 and Figure 7-2 of /SKB, 2004b/.

Repository depth	500 m
Canister spacing	7.5 m
Rock thermal conductivity	2.74 W/(m·K)
Rock heat capacity	2.24 MJ/(m³K)
Temperature at repository depth	14.8°C

Sensitivity analyses

The three rock domains used for canister deposition in layout D1 have average rock thermal conductivities of 2.8, 2.74 and 2.74 W/(mK), respectively, obtained from a number of mineral samples from each rock domain. The above central case uses the lower of these average values, i.e. 2.74 W/(mK). Figure 3-9 shows the effects of varying the rock thermal conductivity. As can be seen from the figure, the temperature criterion for the canister surface would be violated for canisters deposited where the thermal conductivity is below about 2.5 W/(mK), i.e. about one standard deviation below the average value suggested in the site description, see Table 3-7. As already discussed, the scaling of thermal conductivity is uncertain, but these results imply that the canister spacing suggested by design may be insufficient at some canister locations.

Figure 3-10 shows how the peak temperatures vary with the centre-to-centre spacing of the canisters. This distance is controlled by the implementer and is thus not uncertain in the same sense as e.g. the rock thermal conductivity discussed above. It is important to carefully select an appropriate spacing, since this determines the overall requirements on space for the deep repository.

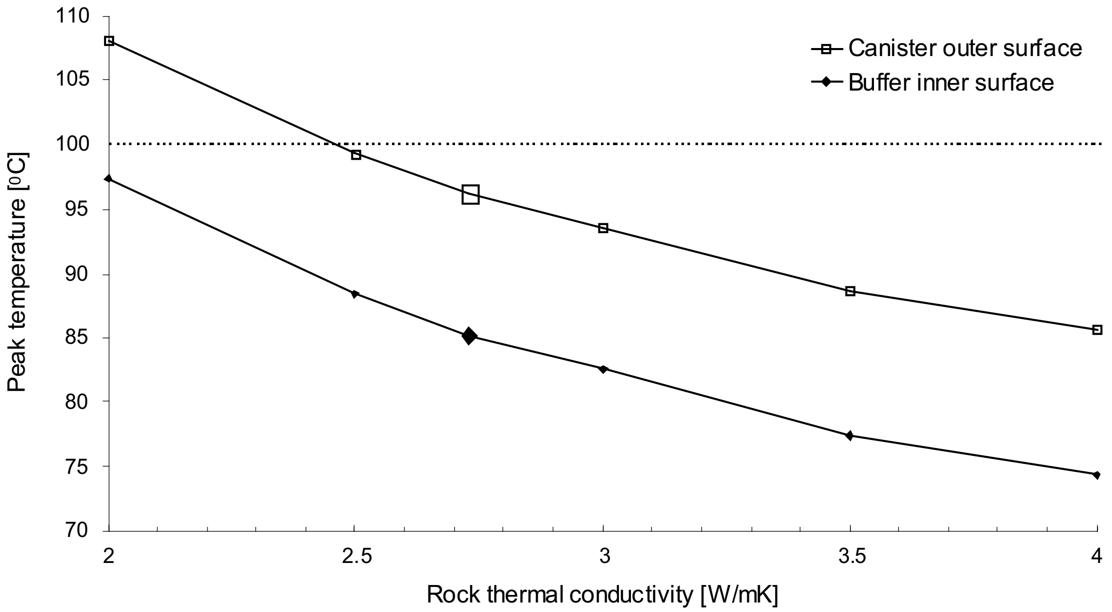

Figure 3-9. Sensitivity of canister and buffer peak temperatures to the rock thermal conductivity. Other data as in Table 3-7.

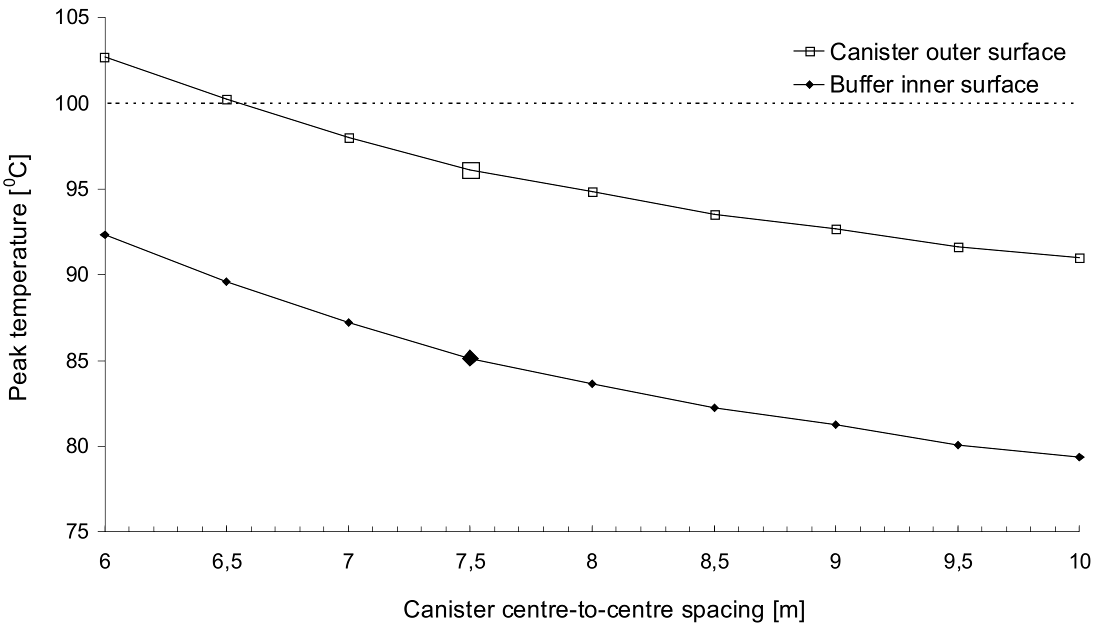

Figure 3-10. Sensitivity of canister and buffer peak temperatures to the canister centre-to-centre spacing. Other data as in Table 3-7.

3.4.4 Safety implications

The previous sections show that the Simpevarp subarea meets all thermal *requirements and preferences*.

It is possible to define a layout that ensures that the required temperature conditions on canister and buffer are fulfilled. However, the spatial variability of the thermal conductivity may be too large for the currently adapted design rules. The additional temperature analyses reported here imply that the canister spacing now suggested by design may be insufficient at some canister locations. Increasing the canister spacing would alleviate this problem and it is important to carefully select an appropriate spacing since this determines the overall requirements on space for the deep repository.

The temperature margin for gaps and uncertainty/variability in rock thermal conductivity applied in the design work should be revisited, since the present rules seem to leave too little margin for these factors. It could also be noted that the fact that some deposition holes will be discarded, would of course reduce the temperature load in the vicinity of these discarded holes, but has little impact on the maximum temperature seen by an average canister. Most canisters will be located at the minimum distance separation and the maximum temperature depends primarily on the local loading conditions.

Even if the thermal requirements and preferences are met, further reduction of uncertainties in the spatial variability and scaling of thermal conductivity would allow for a more efficient design. Increasing canister spacing 1 m implies about 12 percent increase in deposition area. Reducing the uncertainties could also improve the safety case, as there would be less strict demands on the layout in order to meet the temperature requirements. Such a reduction could be made through the methods envisaged in Chapter 12 and 13 in SDM S1.2, both as regards measurement and modelling.

3.5 Hydraulic analyses

The hydraulic properties of the rock, i.e. the permeability and conductivity of the fracture systems, control the amount, rate and distribution of the groundwater flow in the rock. Groundwater flow is important for safety, since groundwater flow is essentially the only pathway through which radionuclides could migrate from potentially breached canisters into the biosphere. Groundwater flow also affects the composition of the groundwater in a potential repository volume and hence the stability of the engineered barriers.

3.5.1 Criteria and other safety considerations

Previously set criteria

The suitability criteria, as set out by SKB in /Andersson et al. 2000/, directly related to the hydraulics of the site concern the permeability (or rather transmissivity distribution) of fracture zones and of the fractures.

Generally, low groundwater flow implies more stable chemical conditions and better retention of radionuclides compared to a situation with high groundwater flow. It is therefore a *requirement* that deposition holes are not positioned too close to regional or local major fracture zones. An exception can be made from this requirement if it can be shown that the permeability of the zone does not deviate significantly from that of the rest of the rock mass.

It is stated as an advantage (i.e. *preference*) if a large portion of the rock mass in the deposition area has a hydraulic conductivity $K < 10^{-8}$ m/s (on a 30 m scale) as such low conductivity would imply high "transport" resistance or F-values (see section 3.7.3). From a repository engineering perspective it is also advantageous with low hydraulic conductivity in the deposition holes, as this would limit the inflow of water in the deposition holes during deposition, thus clearly simplifying the deposition procedures.

A simple motivation for this *preference* value is also suggested in the suitability criteria document /Andersson et al. 2000/. In a homogeneous porous medium $F = a_r L/q$ and $q = -K\text{grad}(H)$, where a_r is the flow-wetted surface area per volume of rock, L is the transport pathway lenght, q the Darcy velocity, K the hydraulic conductivity and grad(H) the gradient of the groundwater head. If it is assumed that grad(H) is 1 percent, L is 30 m (i.e. a distance generally shorter than the respect distances to the deformation zones as applied by rock engineering) and a_r is approximately 1 m^2/m^3, then $F > 10^4$ y/m if $K < 10^{-8}$ m/s. It was noted in SR 97 /SKB, 1999b/ that such high F-values imply substantial retention in the rock. For these reasons, /Andersson et al. 2000/ suggest that during the site investigation a large portion of interpreted hydraulic conductivity values in the rock mass should have a hydraulic conductivity $K < 10^{-8}$ m/s. Otherwise, there would be a need for local detailed adaptation of the design if the safety margin is to be met.

For repository engineering considerations, it is also stated that deformation zones that need to be passed through during construction should have such low permeability that passage can take place without problems. This would generally mean zones with transmissivity $T < 10^{-5}$ m^2/s or zones that are not wide and clay-filled. If such zones are encountered during the site investigation there should be an increased attention to impacts of and problems with grouting and other construction-related risks.

The groundwater flow is also determined by the driving force, which can be expressed as the hydraulic gradient for non-saline groundwater. Data on the hydraulic gradient, boundary conditions, or data on recharge/discharge areas primarily are needed for building credible groundwater models, and not for setting criteria. No requirements were set, but rather arbitrarily it was suggested that there is an advantage if the local gradient is less than 1 percent at repository level (but no additional advantage if even lower) and that areas with an unsuitably high gradient (much greater than 1 percent) should be rejected during the feasibility study phase. However, during the site investigation phase, supporting data are mainly used to build credible models and are not part of the suitability criteria.

Additional considerations

As already explained above the preference values for hydraulic conductivity on the canister scale are based on rather simplistic reasoning. If anything, the suggested limits appear a little pessimistic.

A more useful criterion would be the distribution of Darcy velocity and transport resistance F along potential migration paths. A full assessment of these entities is rather resource demanding and could only be meaningfully carried out within a safety assessment. However, estimates of the distribution of these quantities using the regional-scale numerical groundwater flow model developed as a part of the SDM is more straightforward. Such an analysis is reported in section 3.7.

3.5.2 Hydraulic properties and effective values of permeability

As further explained in Chapter 8 of SDM S1.2, the conceptual hydrogeological model of the site implies that only fractures and fracture zones could conduct water, although the rock matrix may be connected to the flow system by diffusion. In model the conductive features are divided between Hydraulic Conductor Domains (HCD), which essentially coincide with the deformation zones in the geological model, and the Hydraulic Rock Domains (HRD) representing the rock mass between the HCDs. The hydraulic properties of the HR Ds are modelled as discrete fracture network models, with the geometry taken from the geological discrete fracture network model, but with added hydraulic properties. The models are calibrated against existing hydrogeological borehole data.

Transmissivity of the deformation zones

The HCDs in the hydrogeological model are based on the SDM S1.2 regional-scale deformation zones, see section 3.2.4. Some of the zones in the regional-scale model area, particularly in the vicinity of Äspö Island, are to be considered as high-confidence zones (concerning their existence) and several of them have been hydraulically tested. However, most HCDs have been assigned highly uncertain hydraulic properties.

For 13 of the deformation zones there are identified intersections with boreholes. These intersections have been hydraulically tested. The range of the interpreted transmissivity (T) for these HCDs is 1×10^{-8} to 3.6×10^{-4} m^2/s (see Table 8-13 in SDM S1.2).

The geometric mean of the transmissivity of HCDs from the Äspö HRL is $T = 1.3\times10^{-5}$ m^2/s with a standard deviation $Log_{10}T = 1.55$ /Rhén et al. 1997/. This geometric mean T was assigned to all the rest of the HCDs in the regional scale model, regardless of their geological genesis. However, confidence in these values is low, since measurements are lacking. However, it is encouraging that the calibration of the regional groundwater flow model did not entail modification of the transmissivity of the HCDs. Similarily, no such modification was required for the Hydro-DFN models, see next subsection.

The impact of the uncertainty on regional flow and evolution of groundwater composition is assessed in the numerical regional flow modelling by exploring cases with varying numbers of deformation zones, see also section 3.5.3 below.

Hydraulic properties of the rock mass

The hydraulic properties of the rock mass are described by means of a hydraulic discrete fracture network model (Hydro-DFN). As already discussed in section 3.2.4 above, the hydrogeological teams developed their own alternative of the geological DFN model, which better matched the measured intensity of subhorizontal fractures measured in the boreholes. Then, in an additional step, the model is developed by attributing a transmissivity distribution to the fractures.

The working hypothesis embedded in the Hydro-DFN model employed for Simpevarp S1.2 is that it couples an inferred power-law size distribution of fractures, up to the size of local minor fracture zones, to hydraulic properties by applying various alternative hypotheses. The basic hypothesis is to assume that the transmissivity value is dependent on the size through a power-law relationship, but alternatives without any correlation or with only a statistical size-transmissivity correlation were also assessed. Some different geometrical variants were also explored. Furthermore, two modelling teams made the assessment. These teams analysed some common cases, for benchmarking, and also assessed individual cases, see Chapter 8 of SDM S1.2.

Calibrating the different models to the flow data measured in the boreholes results in a number of alternative Hydro-DFN models that all match the data. This is also true when applying the different models in regional flow simulations and trying to match the measured salinity distribution of the site, see also section 3.5.2. The corresponding model parameters are illustrated for the correlated case in Figure 3-11 and given in full in Tables 8-16 and 8-17 of SDM S1.2.

Table 3-10 shows the resulting volumetric fracture intensity for all ("total") fractures, P_{32T}, and the volumetric fracture intensity for all conductive and hydraulically connected fractures P_{32C}, as calculated by the two modelling teams (CF and DT), see /Hartley et al. 2005/ and /Follin et al. 2005/. P_{32c} is obtained by calibrating the DFN-model to ensure that the simulated frequency of flowing and connected fractures intersecting boreholes agrees with the measured frequency of flowing features, see further the discussion in section 8.5.3 of SDM S1.2.

Uncertainties in the hydraulic DFN-model originate from the uncertainty in the geological DFN-model (see above) and the uncertainty in the transmissivity distribution between and within fractures and features. The latter uncertainty is due to relatively few measurements, the indirect characterising of the measurement methods (Posiva Flow Log, PFL and the Pipe String System, PSS), and the uncertain conceptual models for coupling transmissivity as a function of feature size. Connected to this is the fact that the larger features of the DFN-model in reality usually are made up of many small fractures, although they are represented as a single feature in the model. The relatively high and varying measurement limit of the PFL also adds uncertainty of the low permeability end of the transmissivity distribution. However, assessment with different alternative models should ensure good capture of the uncertainty range. Furthermore, the fact that two independent teams have assessed the data should enhance the quality and reliability of the assessment.

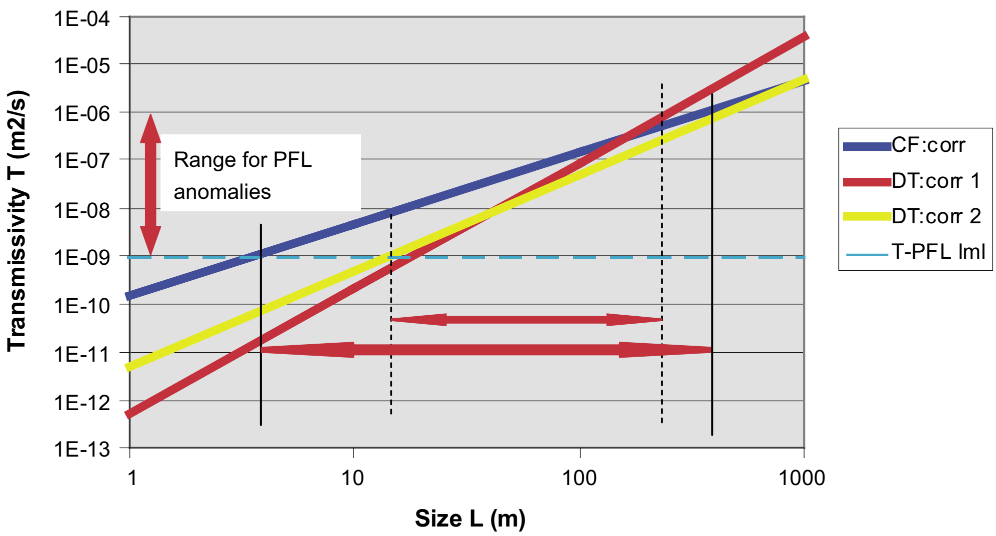

Figure 3-11. *T vs L for the base case as recommended by the two teams (DT and CF). PFL stands for the Posiva Flow Log measurement method (Figure 8-21 in SDM S1.2).*

Table 3-10. Volumetric fracture (feature) intensity for all ("total") fractures, P_{32T}, and volumetric fracture (feature) intensity for all conductive and hydraulically connected fractures P_{32C}, as calculated by the two modelling teams (CF and DT) and scaled to a common minimum size, based on Table 8-18 in SDM S1.2.

Modelling team	Size interval (m)	P_{32T} (m^2/m^3)	P_{32C} (m^2/m^3)
CF	0.5–1,000	0.71	0.29
DT (2)	0.5–300	0.77	0.29

Effective values of permeability

The different alternative Hydro-DFN models have been used to simulate effective values of hydraulic conductivity at different scales. The simulations are essentially set up by generating discrete fractures in large blocks, applying simple boundary conditions, solving the groundwater flow and then averaging over different block sizes, see Figure 3-12. For modelling reasons it was decided to assess block properties at 20 m and 100 m scale, rather than at the 30 m scale set out in the criteria, but the 20 m scale values give a good representation also of the 30 m scale.

Table 3-11 summaries the results of the block modelling. As can be seen from the table, the 20 m scale blocks are on average less permeable than 10^{-8} m/s but, depending on the conceptual model studied, there is a spatial variation and some blocks have higher hydraulic conductivity.

Despite the rather high uncertainties in the Hydro-DFN properties, it is likely that the uncertainty is less in the block properties since they represent averages and since they all are matched with the same hydraulic data. The span given by the different alternative models would thus probably not underestimate the uncertainty.

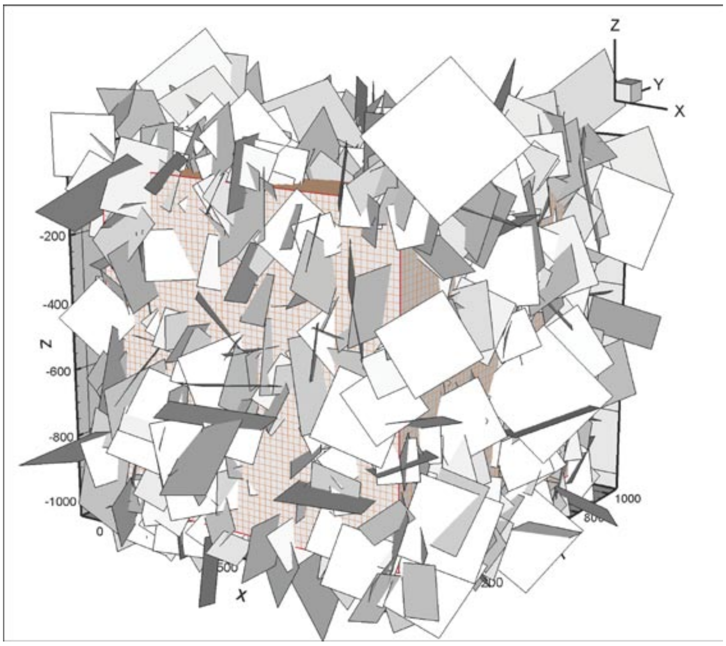

Figure 3-12. *The Hydro-DFN model is used to calculate the block properties at different scales, from /Follin et al. 2005/ (also Figure 8-22 in SDM S1.2).*

Table 3-11. Resulting block properties from the two teams (DT and CF) and for the cases with and without correlation between fracture size and transmissivity. (Table is compiled from Figure 8-23 and Table 8-19 of SDM S1.2).

Case	Scale (m)	Mean Log_{10} (K)	Standard deviation of Log_{10} (K)	Percentage of blocks with $K > 10^{-8}$ m/s
DT Correlated	20	–8.8	1	na
DT Correlated	100	–8.2	0.6	na
CF Correlated	20	–8.5	1.1	40
CF Uncorrelated	20	–8.5	1.4	20
CF Correlated	100	–8.2	0.6	50
CF Uncorrelated	100	–8.9	1.3	5

3.5.3 Groundwater flow calculations and particle discharge points

Based on the hydraulic property description, the SDM S1.2 also presents transient, density dependent groundwater flow calculations in a regional scale. The modelling is performed in two main phases:

- Part 1: Model the groundwater flow from the last glaciation up to present-day with different boundary conditions and hydraulic properties, and compare with measured Total Dissolved Solids (TDS) and interpreted mixing fractions. Part of the purpose is to justify the size of the model and the character of the applied boundary conditions. Also, the effects of discretisation could be tested and help determine an appropriate grid size and assigned grid properties.
- Part 2: Select representative cases from Part 1 and perform flow-path calculations based on the present boundary conditions.

The analyses were performed by the two different modelling teams /Hartley et al. 2005/ and /Follin et al. 2005/ using different numerical codes and somewhat different approaches. The primary concepts used in this regional-scale groundwater flow modelling are that:

- The properties of the hydraulic rock domain (HRD) are represented as a spatially varying equivalent porous medium with properties obtained by upscaling the Hydro-DFN as described in section 3.5.2 above.
- For the hydraulic conductor domains (HCD), i.e. the deformation zones, the properties (transmissivity, thickness, and porosity) are constant over each deformation zone.
- The boundary conditions on the sides are no-flow and zero flux of reference waters. On the bottom of the model at z = −2,300 m, there is a no-flow condition. Different locations of the boundaries are tested.
- Different initial conditions for the salt water distribution and water types at the end of the last glaciation are tested. A fit of simulated results to available measured data was obtained by employing freshwater conditions, mainly of glacial type, down to c. 700 m depth, with a linear increase of salinity down to 1,500 m. No other set-ups of the water types were assumed as initial conditions. All other water types were imposed at the upper boundary as a function of time, based on the shore-line displacement due to the land uplift.

For more detail, see section 8.4 of SDM S1.2, /Hartley et al. 2005/ and /Follin et al. 2005/.

/Hartley et al. 2005/ also calculated flow paths representing the present-day flow conditions, i.e. 2,000 AD, by using the results of the final time-step in the simulations. The analyses are made by particle tracking, with particles released from an area located within the Simpevarp subarea at 500 m depth, see Figure 3-13. It is found that the released particles rapidly reach a HCD and subsequently follow the system of HCDs to discharge points below the Baltic Sea. The discharge points for release in the Simpevarp subarea are found to the south and east of the subarea, as expected, see Figure 3-14.

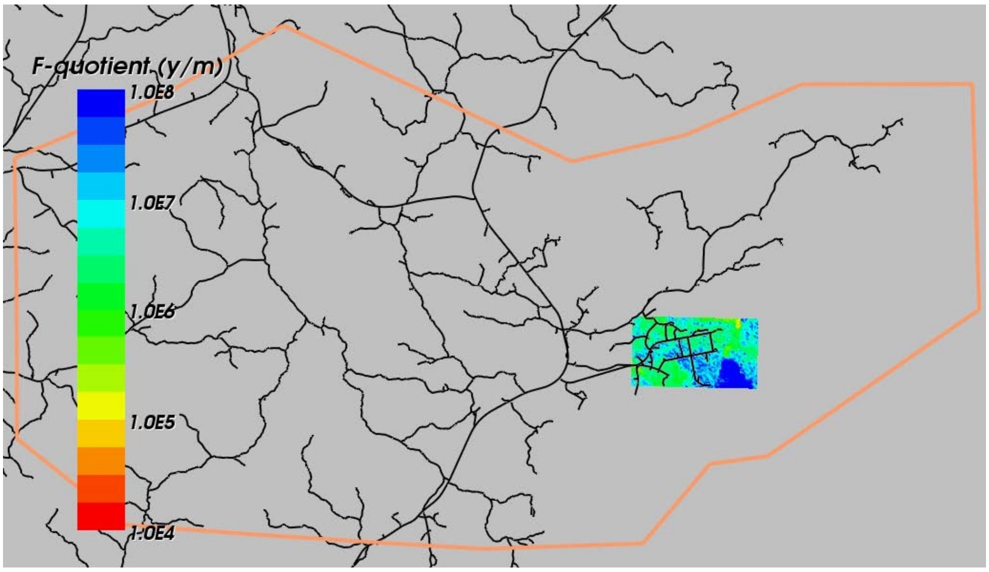

Figure 3-13. *Particle starting locations from the Simpevarp subarea. Roads are shown in black for context. (From /Hartely et al. 2005/, Figure 9-3).*

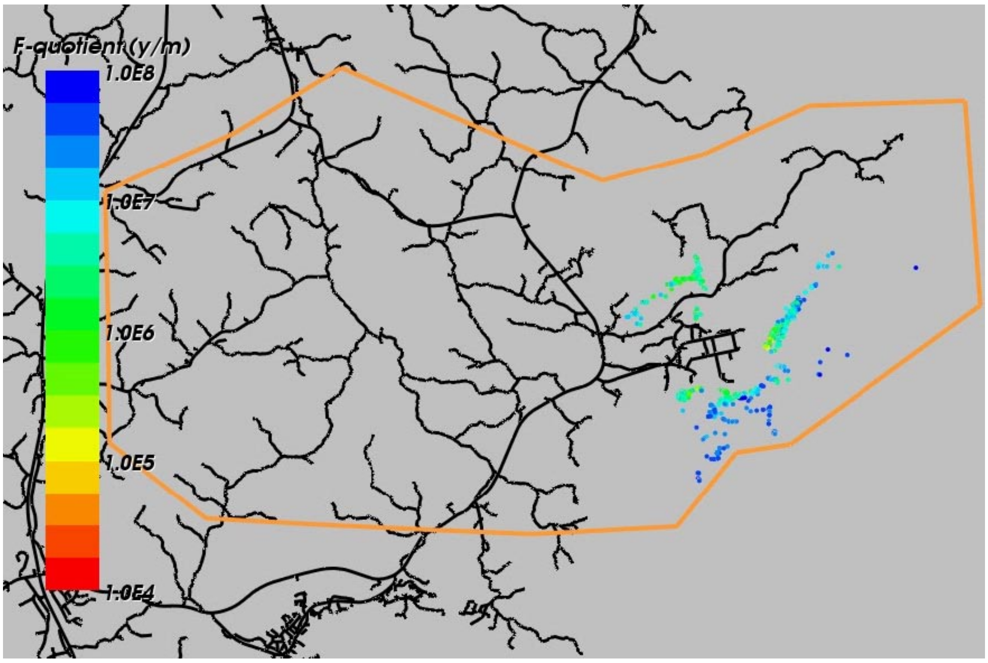

Figure 3-14. *Particle exit locations from the Simpevarp subarea release for the Base Case (SReg_4Component_ IC2). Roads are shown in black for context. (From /Hartley et al. 2005/, Figure 9-5).*

Apart from the base case, several variants, including the alternative models for transmissivity versus size correlations, were tested. These variants comprise:

- Two additional and different realisations of the base case.
- Larger regional domain (LReg_4Component_IC2).
- Hydro-DFN based on DarcyTools interpretation (SReg_4Component_DT_IC2).
- Uncorrelated transmissivity distribution (SReg_4Component_UnCorr_IC2).
- Semi-correlated transmissivity distribution (SReg_4Component_Semi_ IC2).
- Only included HCDs with high confidence of existence and those in Length Classes 2 and 3 (L > 1,500 m) (SReg_4Component_IFZ2_IC2).
- Only included HCDs with high confidence of existence and those in Length Class 3 (L > 3,000 m) (SReg_4Component_IFZ3_IC2).
- Reduced hydraulic conductivity linearly with depth (SReg_4Component_DepthK_IC2).
- Increased hydraulic conductivity in top 100 m (SReg_4Component_K100m_IC2).

Most of these variants show very similar results, both for the flow distribution and exit locations. It should be noted that excluding HCDs smaller than 3,000 m (but including HCDs that were considered certain by the geologists) have only a minor effect on the flow field compared with the case including all deformation zones as HCDs. The reason is that the remaining HCD are still rather many, well-connected and with fairly high transmissivities in the area of interest. In contrast, even a small decrease in K (a factor of 5) significantly changes the flow distribution. Due to the decrease in Darcy velocities, the brine then stays deeper in the model and the flow is shallower. However, the simulated exit locations are not much different from those in the other cases explored.

In SDM S1.2 the regional scale boundary and initial conditions are uncertain. However, the sensitivity analyses conducted by /Hartley et al. 2005/ and discussed above, suggest that these uncertainties are of less concern for the flow field in the Simpevarp subarearea, although they could still affect predictions of long-term groundwater composition.

3.5.4 Safety implications

The previous sections show that the Simpevarp subarea meets all hydraulic requirements. Also, the preferences are judged to be met, although the relatively high and uncertain permeability distribution at potential repository depth should be noted:

- The requirement that deposition holes should not be positioned near regional or local major fracture zones is fulfilled by the geological requirement (see section 3.2).
- As seen in section 3.5.2, between 60 and 80 percent of blocks at the 20 m scale have an effective hydraulic conductivity $K < 10^{-8}$ m/s. Similar, but slightly lower percentages would result if the evaluation had been made at the 30 m scale. The estimate depends on the conceptual model for the hydraulic discrete fracture network model. This means that there could be some uncertainty whether the preference on low hydraulic conductivity is met. However, as explained above, the preference values for hydraulic conductivity at the canister scale are based on rather simplistic reasoning. A more useful criterion would be the distribution of Darcy velocity and transport resistance, F, along potential migration paths, but in the PSE it is only feasible to present estimates of the distribution of these quantities using the regional scale numerical groundwater flow model, see section 3.7.

- The transmissivity range of the HCDs lies between 1×10^{-8} and 3.6×10^{-4} m^2/s. This means that there are a few deformation zones with transmissivity, T, above 10^{-5} m^2/s. If there is a need to pass through these zones during the access tunnel construction, the engineering implications will have to be carefully assessed.
- Particle tracks indicate that the Simpevarp subarea is a local recharge area and flow paths from the repository depth discharge below the sea (see Figure 3-14). The groundwater flow rate is low, indicating low gradients and much below 1 percent at repository level. Furthermore, a sensitivity study shows a very limited impact on these results from various positions of the model boundaries or from the details of the HCD deformation zones in the regional domain.

The rather high level of hydraulic conductivity and uncertainties in the spatial variation and upscaling, warrant further studies. This would both involve collection of additional data, in order to assess potential differences between different rock domains and to better understand potential anisotropy, and additional efforts in evaluating these data. More detailed suggestions for how to reduce the uncertainties are given in the SDM S1.2.

3.6 Hydrogeochemistry

A stable and suitable groundwater composition is a prerequisite for the long-term stability of the copper canister and the bentonite buffer. Thus, the hydrogeochemistry directly affects the potential for isolation.

3.6.1 Criteria and other safety considerations

Previously set criteria

The suitability criteria, as set out by SKB in /Andersson et al. 2000/, directly related to the chemical conditions of the site essentially concern dissolved oxygen, pH, salinity or Total Dissolved Solids (TDS) and some other chemical parameters.

It is a *requirement* that the groundwater at repository depth does not contain dissolved oxygen at repository level since dissolved oxygen could corrode the copper canister and thus threaten containment. Groundwater with negative Eh, occurrence of Fe(II) or with occurrence of sulphide (HS^-) cannot, for chemical reasons, contain dissolved oxygen, which means that the requirement is fulfilled if any of these indicators are present over the proposed repository domain. As a criterion for the site investigations it is stated that groundwater from potential repository depth must exhibit a least one of these indicators. Otherwise the site should be abandoned.

The groundwater pH affects the stability of the bentonite and also affects retention properties (sorption and solubilities). There is no requirement, but there is a *preference* that undisturbed groundwater at repository level should have a pH in the range 6–10. This is assessed by checking whether quality assured groundwater samples taken below the 100 m level lie within the preferred range.

Groundwater salinity affects bentonite swelling. At the time of publishing the suitability critera, experimental evidence led to a *required* limit of TDS < 100 g/L in order to ensure sufficient bentonite swelling. During site investigations quality-approved measured TDS at repository level must meet this requirement. Occasional higher values can be accepted if it can be shown that the water is located in areas that can be avoided.

There are also *preferences* set for some other chemical parameters in the deep groundwater, namely [DOC] < 20 mg/L[3], colloid concentration < 0.5 mg/L, low ammonium concentrations, $[Ca^{2+}]+[Mg^{2+}] > 4$ mg/L at repository depth and low concentrations of Rn and Ra. These preferences are set to ensure limited concern for organic matter, ensure no colloid enhanced transport, ensure no colloid generation from the buffer and to ensure safe working conditions underground. If concentrations measured during the site investigation deviate from preferences the safety implications need to be specifically assessed.

Additional consideration

The SR-Can Interim report /SKB, 2004b/ states that the total concentration of divalent cations should exceed 1 mM, i.e. around 40 mg/L, in order to avoid chemical erosion of buffer and backfill. This is a stricter condition than the one mentioned above. Also, it should be noted that SR-Can intends to carry out a detailed evaluation of the different potential backfill materials and how they would be affected by different salinity levels.

Furthermore, the redox buffering capacity of the geosphere may be evaluated from detailed mineralogy evaluations of the rock types listed in Table 3-3, as well as of the fracture-filling minerals. The redox parameters of interest are Fe(II) and sulphide content. The redox buffering capacity is of importance when evaluating the impact of the operational phase. In case of a glaciation, the effects of introducing glacial melt water, that may be oxygen-rich, would also depend on the redox buffering. Similarly, the pH-buffering capacity may be also evaluated from the amounts of calcite in the fractures. Detailed mineralogical data are not available for the SDM S1.2, and therefore this aspect of the site geochemistry cannot be evaluated at this stage.

3.6.2 Current groundwater composition

According to the conceptual hydrogeochemical model of SDM S1.2, local groundwater flow regimes are assumed to develop in the Laxemar and Simpevarp subareas and are considered to extend down to depths of around 600–1,000 m, depending on local topography. Close to the Baltic Sea coastline, where topographical variation is small, the depth of the penetration of local groundwater flow will be less marked. In contrast, the Laxemar subarea is characterised by higher topography resulting in a much more profound groundwater circulation, which appears to extend to 1,000 m depth in the vicinity of borehole KLX02.

The marked differences in the groundwater flow regimes (in terms of depth penetration of local flow cells) between the Laxemar and Simpevarp areas are reflected in the groundwater chemistry. Figure 3-15 shows four major recognised hydrochemical groups of groundwaters denoted by A–D. The main features of the four identified groundwater types are summarised below.

TYPE A: Shallow (< 200 m) at Simpevarp but deeper (0–900 m) at Laxemar. Dilute groundwater (< 1,000 mg/L Cl; 0.5–2.0 g/L TDS) Mainly Na-HCO_3 in type. Redox: Marginally oxidising close to the surface, otherwise reducing. Main reactions: Weathering; ion exchange (Ca, Mg); dissolution of calcite; redox reactions (e.g. precipitation of Fe-oxyhydroxides); microbially-mediated reactions. Mixing processes: Mainly meteoric

[3] In /Andersson et al. 2000/ it was only stated that DOC concentrations at depth should be low, the value of 20 mg/L has later been decided to be a reasonable preferred upper limit. /Andersson et al. 2000/ also suggest that [DOC] > 10 mg/L in surface waters.

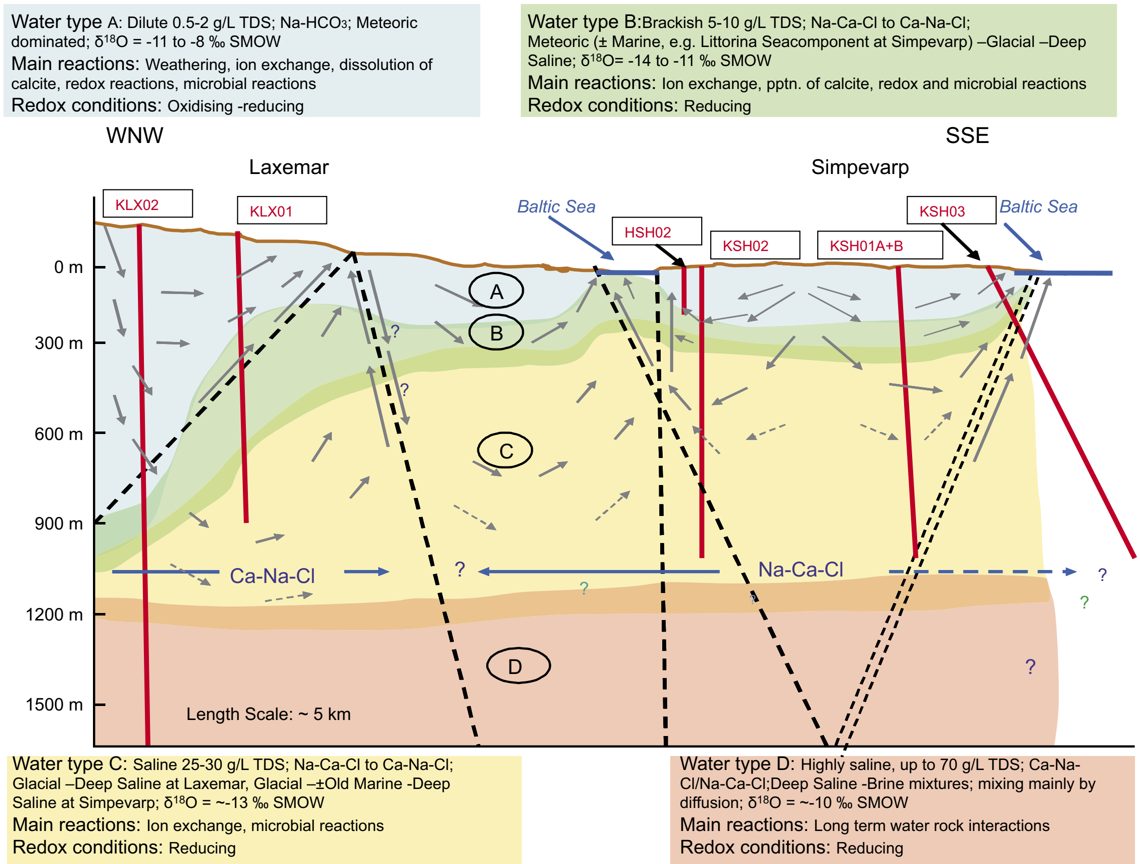

Figure 3-15. *Schematic conceptual hydrogeochemical model based on integrating the major structures, the major groundwater flow directions and the different groundwater chemistries (A–D) and properties. The dashed black lines indicate deformation zones. (Figure 11-11 in SDM S1.2).*

recharge water at Laxemar; potential mixing of recharge meteoric water and a modern sea component at Simpevarp; localised mixing of meteoric water with deeper saline groundwaters at Laxemar and Simpevarp

TYPE B: Shallow to intermediate (150–300 m) at Simpevarp, but deeper (approx. 900– 1,100 m) at Laxemar. Brackish groundwater (1,000–6,000 mg/L Cl; 5–10 g/L TDS). Mainly Na-Ca-Cl in type, but some Na-Ca(Mg)-Cl(Br) types at Simpevarp; transition to more Ca-Na-Cl types at Laxemar. Redox: Reducing. Main reactions: Ion exchange (Ca, Mg); precipitation of calcite; redox reactions (e.g. precipitation of pyrite), microbial reactions Mixing processes: Potential residual Littorina Sea (old marine) component at Simpevarp, usually in fracture zones close to or under the Baltic Sea; meteoric and potential glacial component at Simpevarp and Laxemar; potential deep saline (nonmarine) component at Simpevarp and at Laxemar.

TYPE C: Intermediate to deep (> 300 m) at Simpevarp but deeper (approx. 1,200 m) at Laxemar. Saline (6,000–20,000 mg/L Cl; 25–30 g/L TDS) Mainly Na-Ca-Cl with increasingly enhanced Br and SO_4 with depth at Simpevarp; mainly Ca-Na-Cl with increasing enhancements of Br and SO_4 with depth at Laxemar. Redox: Reducing. Main reactions: Ion exchange (Ca), microbial reactions. Mixing processes: Potential glacial component at Simpevarp and Laxemar; potential deep saline (i.e. non-marine and/or non-marine/old Littorina marine) component at Simpevarp, deep saline (non-marine) component at Laxemar.

TYPE D: Deep (> 1,200 m) only at Laxemar: Highly saline (> 20,000 mg/L Cl; to a maximum of ~ 70 g/L TDS) Mainly Ca-Na-Cl with higher Br but lower SO_4 compared with Type C groundwaters. Redox: Reducing. Main reactions: Water/rock reactions over long residence times, microbial reactions. Mixing processes: Probably long term mixing of deeper, non-marine saline component driven by diffusion.

For current conditions the groundwater at the Simpevarp subarea is of type C at the potential repository levels. Table 3-12 presents analysed values of a representative sample at potential repository level in the Simpevarp subarea: i.e. KSH01A:548–565 m and KSH02:575–580 m, for the chemical parameters included in requirements and preferences.

As can be seen from the table there are no analyses of colloid content in these boreholes, but colloid levels are measured in KLX01 in the Laxemar subarea and in KAV01 at Ävrö. In SDM S1.2, Chapter 11 it is noted that the number of colloids decreases with depth in KLX01 but not in KAV01. The average concentration of colloids in this study is $63 \pm 49\ \mu g\ L^{-1}$ and is in agreement with colloid studies from Switzerland (30 ± 10 and $10 \pm 5\ \mu g\ L^{-1}$) and Canada ($300 \pm 300\ \mu g\ L^{-1}$) where they used the same approach as in the Simpevarp area /Laaksoharju et al. 1995/.

The main uncertainties in the version 1.2 hydrogeochemical model are:

- Spatial variability in 3D at depth.
- Groundwater composition in the rock matrix.
- Temporal (seasonal) variability in surface water chemistry, which ultimately impacts the groundwater in the bedrock.
- Model uncertainties (e.g. equilibrium calculations, migration and mixing).
- Identification and selection of end-member waters. This is a judgemental aspect of the M3 (principal components) analysis.

There is uncertainty in spatial variability in 3D at depth, as the information density concerning borehole groundwater chemistry is low. The uncertainty in spatial distribution is quantified with a local uncertainty in the order of ± 50 percent and a site-scale uncertainty in the order of ± 10 percent, see section 9.6 of SDM S1.2.

Table 3-12. Analysed values of represenative sample at potential repository level in the Simpevarp subarea: i.e. KSH01A:548–565 m and KSH02:575–580 m, for the chemical parameters included in requirements and preferences, (Table 11-7, in SDM S1.2).

	Eh (mV)	pH (units)	TDS (g/L)	DOC (mg/L)	Colloids (mg/L)	Ca+Mg (mg/L)
Criterion	< 0	6–10	< 100	< 20	< 0.5	> 40
KSH01A:548–565 m	–230	7.6	15.1	< 1	NA	1,947
KSH02:575–580 m	NA	8.1	14.1	< 1	NA	1,797

NA = Not analysed

3.6.3 Safety implications

The previous sections show that the Simpevarp subarea meets all hydrogeochemical requirements and preferences:

- Table 3-12 shows that the groundwater composition sampled at potential repository depth in the Simpevarp subarea lie well within both the required and preferred bounds. Even if there are no data on colloid levels from these samples – other data from the site though show that the colloid levels are sufficiently low.
- Furthermore, even if the exact spatial distribution of the water composition is uncertain, all the four water types identified conform to the hydrogeochemical criteria. Specifically, there is no indication of dissolved oxygen at depth and TDS levels range from 0 to at most 70 g/L. This also means that even if the exact future evolution of groundwater composition is uncertain, due to uncertainties in future groundwater flow, it is highly likely that the groundwater composition will remain within the range of the required and preferred criteria also in the future.

However, even if the hydrogeochemical requirements and preferences are met, further reduction of uncertainties would further improve the understanding of the hydrogeochemistry and would thus enhance the safety case. The additional data and evaluations suggested for this in SDM S1.2, continue to seem appropriate. As already mentioned, SR-Can also intends to carry out a detailed evaluation of the different potential backfill materials and of how different salinity levels would affect them. This evaluation might also result in further needs for a more detailed evaluation of the present and a prediction of the future salinity distribution at the site. Furthermore, in order to evaluate the redox buffering capacity of the geosphere, detailed mineralogical data on Fe(II) and sulphide content of the rock and fracture minerals would be needed.

3.7 Radionuclide transport

The only pathway through which radionuclides could migrate from potentially breached canisters into the biosphere is through groundwater flow. That migration, and the retardation of the migration, is controlled by the distribution of the groundwater flow and the migration properties of the rock matrix along the migration paths.

3.7.1 Criteria and other safety considerations

Previously set criteria

The suitability criteria, as set out by SKB in /Andersson et al. 2000/, directly related to the transport properties of the site concern the flow-related transport properties, i.e. groundwater flow (Darcy velocity) at canister scale, transport resistance F, and the migration properties of the rock matrix.

It is *required* that the Darcy velocity at the canister scale and the total fracture aperture are not large enough to damage the bentonite during deposition. However, this can always be controlled and avoided during deposition and is not further discussed here. For safety, there is instead a *preference* for the Darcy velocity, after closure and resaturation, at the canister scale to be less than 0.01 m/y for a large number of positions in the rock since flows less than this helps in limiting the release of radionuclides from the buffer in case the canister is breached. There is also a *preference* that a large fraction of flow paths from potential canister position through the rock should have a transport resistance F > 10^4 y/m, as such high F-values imply significant retention of sorbing radionuclides. However, /Andersson et al. 2000/, also point out that these "limiting" values should be seen as a guideline and that a final judgement of the adequacy of retention is made within the framework of a safety assessment.

Also the migration properties of the rock matrix affect radionuclide retention in the rock. It is a *preference* that matrix diffusivity and matrix porosity are not much lower, i.e. by more than a factor of 100, than the value ranges analyzed in the safety assessment SR 97 (see the SR 97 Data Report /Andersson, 1999/). Also the accessible diffusion depth should at least exceed a centimetre or so. Otherwise, special consideration of the safety implications will be required in coming safety assessments.

Additional considerations

There are no additional considerations. However, it should be noted that the degree of retention of a radionuclide is element specific and that the importance of the retention depends on the release situation and the half-life of the individual radionuclide. Combining all such aspects is an important part of a safety assessment and will be done in SR-Can, but lies outside the scope of the PSE. This also means that the criteria on Darcy velocity and transport resistance should be seen as guiding indications – not as strict rules.

3.7.2 Migration properties of the rock matrix

As further explained in Chapter 10 of SDM S1.2, the site descriptive modelling of transport properties only considers retardation parameters (porosity, diffusivity and sorption coefficient), whereas the flow-related migration properties are handled outside the Site Descriptive Model report. Site investigation data from porosity measurements and diffusion experiments (*in situ* and in the laboratory) have been available for the SDM S1.2 modelling. The modelling work has included evaluations of data on rock mass geology, fractures and fracture zones, and hydrogeochemistry, in addition to the evaluation of transport data.

The retardation model for the rock mass contains data for the fresh and altered forms of the major rock types in the Simpevarp subarea (Ävrö granite, quartz monzodiorite and fine-grained dioritoid). Specifically, the retardation model is based on porosity data from water saturation measurements on site-specific rock samples, diffusivities from formation factors measured in the laboratory, electrical resistivity measurements on site-specific samples, and sorption coefficients imported from the Äspö HRL. The sorption dataset is limited to Cs and Sr under hydrochemical conditions corresponding to "Groundwater type III" (as specified by /Tullborg et al. 2005/). Table 3-13 summarises the mean values and standard deviations (expressed as mean value ± one standard deviation) of the transport parameters of the rock mass.

The main uncertainties in the SDM S1.2 model of the bedrock transport properties concern:

- Site-specific sorption and diffusion parameters.
- Assignment of parameter values to the "elements" in the geological description ("typical" rock materials and structures).
- Understanding of retention/retardation processes as a basis for selection of parameter values in models.
- Correlation between matrix transport properties and flow paths.

Table 3-13. Range of transport parameters for the major rock types in the Simpevarp subarea. (From Table 11-8 in SDM S1.2).

Rock type	Porosity (vol-%)	Formation factor (–)	K_d Sr (m^3/kg) (GW type III)	K_d Cs (m^3/kg)[2] (GW type III)	Comments
Ävrö granite (fresh)	0.40 ± 0.13	$(2.9 \pm 2.9)\cdot 10^{-4}$	$(4.2 \pm 0.8)\cdot 10^{-5}$	0.06 ± 0.03	Dominant rock type in RSMA01. One of the two dominant rock types in RSMC01.
Quartz monzo-diorite (fresh)	0.20 ± 0.13	$(1.1 \pm 1.6)\cdot 10^{-4}$	$(4.2 \pm 0.8)\cdot 10^{-5}$	0.06 ± 0.03	One of the two dominant rock types in RSMC01.
Fine-grained dioritoid (fresh)	0.17 ± 0.15	$(1.0 \pm 1.7)\cdot 10^{-4}$	$(4.2 \pm 0.8)\cdot 10^{-5}$	0.06 ± 0.03	Dominant rock type in RSMB01.
Altered rock	0.33	$(0.8 \pm 0.4)\cdot 10^{-4}$	$(1.2 \pm 0.2)\cdot 10^{-5}$	0.013 ± 0.006	The same parameter values are assumed for the altered forms of all major rock types.

A main reason for these uncertainties is the limited supply of site-specific transport data and that all relevant rock types are not represented in the Äspö data, which could be used as an analogue. There are also limitations in the geological description concerning, e.g. porosity, fracture mineralogy and alteration. However, these uncertainties can still be quantified, as indicated in Table 3-13, using data from various geological environments.

It has also been questioned whether the measurement of the formation factor would be biased due to mechanical unloading of the rock samples. However, an evaluation of the relation (ratio) between laboratory and *in situ* formation factors shows no obvious depth trend that would demonstrate increasing effects of stress release in the laboratory samples. This could possibly be explained by the, relatively speaking, low-stressed rock at the Simpevarp subarea.

3.7.3 Flow related migration parameters

As already discussed in section 3.5.3, /Hartley et al. 2005/ have calculated flow paths from release areas located within the Simpevarp subarea at 500 m depth, based on the hydraulic properties description in the SDM S1.2 and the present day boundary conditions. The particles are released within a rectangle corresponding to the local-scale, Simpevarp release area at –500 m elevation and with a spacing of 50 m, see Figure 3-13.

As a separate effort, and not reported in the SDM S1.2, /Hartley et al. 2005/ also calculated advective travel time (t_w), canister flux (q_c, Darcy velocity), F-value (F) and path length (L) for each of these flow paths, using the following definitions:

- Travel time, $t_w = \sum_l \frac{\phi \delta l}{q}$, where δl is a step in distance along the path, for example through one finite-element, φ is the kinematic porosity, and q the Darcy velocity.

- Canister flux, $q = q_0$, the initial Darcy velocity at the release point.

- Pathlength, $L = \sum_l \delta l$.

- Transport resistance, $F = \sum_{l} \frac{a_r \delta l}{q}$, where a_r is the fracture surface area per unit volume of rock.

In Safety Assessment the Darcy velocity at canister scale and the transport resistance, F, will be calculated from nested Discrete Fracture Network and Equivalent Porous medium flow simulations, where the repository region is described as a DFN at the detailed scale, as already outlined in SR-Can Interim /SKB, 2004b, Chapter 9/. However, this procedure is not possible for the large-scale relatively low resolution analyses carried out in the regional flow modelling. The calculated Darcy velocity will be an average for a larger volume and an effective value of the fracture surface area per unit volume of rock, a_r, is needed in order to assess the transport resistance.

Conceptually, a_r equals the fracture surface area (both faces of the fracture plane) of the hydraulically connected network per unit volume of rock or twice P_{32c}. As can be seen from Table 3-10, P_{32c} is estimated to be about 0.3 m^2/m^3. However, /Hartley et al. 2005/ note that P_{32c} could possibly be higher and lie in the range about 0.3 to 1.0. Hence a_r would then be in the range 0.6 to 2.0 m^{-1}. /Hartley et al. 2005/ selects a value of $a_r = 2\ m^{-1}$ for the further analyses. In trying to match current day water distributions /Hartley et al. 2005/ also considered several alternative values of a_r; 1.0, 0.5, 0.25 and 0.1 respectively, but concluded that the better matches result from the high values of a_r.

Table 3-14 provides a statistical summary of these calculated performance measures for a Base Case (SReg_4Component_IC2), with a_r set to 2 m^2/m^3. The calculations have also been performed for the other variants explored, i.e.:

- Two additional realisations of the Base Case.
- Hydro-DFN based on DarcyTools (SReg_4Component_DT_ IC2).
- Uncorrelated transmisisvity distribution (SReg_4Component_UnCorr_ IC2).
- Semi-correlated transmisisvity distribution (SReg_4Component_Semi_ IC2).
- Only included HCD of high confidence of existence and those within Length Classes 2 and 3 (L > 1,500 m) (SReg_4Component_IFZ2_IC2).
- Only included HCD of high confidence of existence and those within Length Class 3 (L > 3,000 m) (SReg_4Component_IFZ3_IC2).
- Reduced hydraulic conductivity at depth (SReg_4Component_DepthK_IC2) using a hydraulic conductivity that reduces linearly with depth.
- Increased hydraulic conductivity in the top 100 m (SReg_4Component_K100m_IC2).

The differences in the performance measures between the variants considered are generally very low. The case with uncorrelated transmissivity distribution (SReg_4Component_ UnCorr_ IC2) results in slightly longer travel times, smaller Darcy velocity and about 10 percent higher F-values compared with the Base Case. This difference is not larger than the difference between different realisations of the base case, indicating the importance of spatial variability. The other variants are even closer to the Base Case. The limited difference between the variants should perhaps come as a surprise, since all the cases considered have been calibrated against the same hydraulic data in the case of the Hydro-DFN variants, and against the same hydrogeochemistry data. However, one variant that has not been considered here that may have a large effect would be to sample the HCD hydraulic properties stochastically rather than using global median values.

Table 3-14. Statistical summary of the calculated performance measures (t_w, q_c, F and L) for the Simpevarp release-area for the Base Case (SReg_4Component_IC2). From /Hartley et al. 2005, Table B-2/.

Statistical entity	$Log_{10}(t_w)$ $[t_w]$ = years	$Log_{10}(q_c)$ $[q_c]$ = m/y	$Log_{10}(F)$ [F] = y/m	$Log_{10}(L)$ [L] = m
Mean	3.182	−3.390	6.606	3.477
Median	3.179	−3.498	6.553	3.572
5th percentile	2.466	−4.527	5.814	2.883
25th percentile	2.755	−3.910	6.275	3.148
75th percentile	3.561	−2.999	6.946	3.728
95th percentile	4.040	−1.703	7.488	3.965
Std dev	0.508	0.792	0.504	0.348
Variance	0.258	0.626	0.254	0.121
Skewness	0.150	0.759	0.066	−0.372
Kurtosis	−0.651	0.855	0.011	−0.926
Min value	1.806	−5.476	4.788	2.746
Max value	4.871	−0.775	8.337	4.295

There are several uncertainties related to the value of a_r. One important uncertainty is the impact of the averaging resulting from the porous medium description. This will be handled in the detailed-scale DFN-approach planned for the Safety Assessment. Another uncertainty is the degree of channelling. This uncertainty will also be assessed within the Safety Assessment, and is not further discussed in this PSE. Nevertheless, given all these uncertainties, it seems reasonable to at least consider a factor of 10 lower values of a_r as a possibility, even if such low values are not supported by the calibration to the hydrogeochemistry data. The reduction would result in a factor of 10 lower values of F than those presented in Table 3-14.

3.7.4 Safety implications

There are no specific requirements on the transport properties other than that they should be sufficient to provide overall safety. Such an overall requirement would likely be fulfilled by meeting the preferences. The previous sections show that the Simpevarp subarea meets all preferences on transport properties.

- The statistical summary in Table 3-14 shows that the number of starting positions with a calculated Darcy velocity above 0.01 m/year is less than 10 percent. This value is little affected by the different variant cases explored.
- The statistical summary in Table 3-14 also shows that all calculated migration paths have a transport resistance F above 10^4 year/m and that only 5 percent of these paths have a transport resistance F less than 6.5×10^5 year/m. This value is little affected by the different variant cases explored. Furthermore, the 10^4 year/m criterion is fulfilled for more than 95 percent of the migration paths even if the value of a_r is reduced by a factor of 10 (or even 60) in order to account for the uncertainty in a_r.

- The range of transport parameters for the major rock types in the Simpevarp subarea shown in Table 3-13, are well within the ranges considered in SR 97. The SR 97 Data Report /Anderssson, 1999/ suggested a matrix porosity between 5×10^{-3} and 5×10^{-4}, a Formation Factor of 4.2×10^{-5} and a K_d for Sr in the range 0.0001 to 0.05 m^3/kg and K_d for Cs in the range 0.05–0.5 m^3/kg.

The detailed scale DFN-approach planned for the Safety Assessment, will alleviate the averaging uncertainties stemming from the porous medium description. As already stated, it should also be noted that the actual retention of a radionuclide is element specific and the importance of the retention depends on the release situation and the half-life of the individual radionuclide. Furthermore, the site-specific information on the migration properties of the rock needs to be complemented by more generic data and it needs to be considered how they are affected by the conceptual uncertainties in the migration processes. Combining all such aspects is an important part of a safety assessment and will be done in SR-Can, but lies outside the scope of the PSE.

There is also a need to reduce the uncertainty in the site description. Most uncertainties concern the hydrogeological DFN-model, and both additional data and additional evaluation analysis is warranted, see also the final discussion in section 3.5.4. In addition to this there is a need, if possible, to reduce the uncertainty in characterising the effects of channelling. However, this can only partly be achieved by new measurement approaches. Further attention to modelling, with different alternatives and careful scrutiny of assumptions, appears to be the way forward.

It is premature in the PSE to assess potential data needs for improving the description of the migration properties of the rock matrix – or even if such improvements will be needed. More *in situ* data would nevertheless enhance the safety case. Better feedback on this issue will be available in relation to the full migration analysis made within SR-Can.

3.8 Importance of analyses previously foreseen but now omitted from the PSE

In the planning document of the PSE it was envisaged that there would be some analyses in addition to the ones already presented in the previous sections. These analyses were designed to provide further feedback to the continued investigations and site-specific repository design. However, omitting these analyses is judged to have negligible impact on the PSE, although it is important that the analyses are carried out eventually, should the site investigations at the Simpevarp subarea be continued. These additional analyses are briefly outlined below.

3.8.1 Drawdown and upconing

Drawdown of surface water and upconing of very saline water are not considered in the previously set criteria /Andersson et al. 2000/. However, these processes could change the groundwater composition at the repository level and could thus be of importance for safety. The extent of these disturbances depends to a large extent on the amount of grouting made in order to control the inflow to the facility.

Analyses of drawdown and upconing are envisaged in the PSE planning document, but are for practical reasons not reported here. The analyses are part of the final design analyses (Step F) and the results will be reported there. Furthermore, SR-Can will consider the implications of the results of those analyses, though for sites other than the Simpevarp subarea.

3.8.2 Influence of grouting and construction materials

The PSE planning report stated that SR-Site will assess the consequence of grouting and other materials, as estimated by Repository Engineering, in the repository, but also envisaged some initial discussion within the PSE. Estimates of the amounts will be carried out as part of the design work, and evaluations for preliminary values would be of little interest. Instead, SR-Can will be the first instance to assess the consequences of these materials, though for sites other than the Simpevarp subarea.

3.8.3 Transmission calculations and transport modelling

Probabilistic integrated radionuclide transport and dose calculations will be carried out in the full safety assessment SR-Can, but for other sites than the Simpevarp subarea. Such modelling efforts are not included in this PSE, essentially since the results cannot be evaluated without a detailed discussion of input data relating not only to the geosphere but also to system components that are not evaluated within the PSE, e.g. the fuel, the canister, the buffer and the deposition tunnels.

3.8.4 Near-surface hydrology

In the PSE planning document it was envisaged that the PSE would explore the properties of the near-surface hydrology as provided in the Site Description, but no additional modelling was planned. It was suggested that combining results of the hydrogeological analyses of the discharge point distribution (see section 3.5.3), with the current understanding of the near-surface hydrology would provide important feedback to the subsequent characterisation work.

Since the issuing of the PSE planning report, SKB has decided to publish a surface system model description of each site. The surface system description model for the Simpevarp subarea is provided in /SKB, 2005c/. That report provides sufficient feedback on the needs for further characterisation, and additional analyses in the PSE are therefor unnecessary.

4 Conclusions and recommendations

The main objectives of this Preliminary Safety Evaluation of the Simpevarp subarea are (section 1.1):

- to determine whether the feasibility study's judgement of the suitability of the candidate area with respect to long-term safety holds up in the light of the site investigation data,
- to provide feedback to continued site investigations and site-specific repository design and
- to identify site-specific scenarios and geoscientific issues for further analyses.

The fulfilment of these objectives is discussed in the following.

4.1 Overall findings regarding long-term safety

The evaluation in the previous chapter shows that even considering remaining uncertainties, the Simpevarp subarea *meets all safety requirements* set out by SKB in /Andersson et al. 2000/. More specifically:

- It is well established that the Simpevarp subarea does not have any ore potential. The rock type distribution represents typical crystalline basement rock and the remaining uncertainties are of little concern for safety.
- It appears possible to locate a sufficiently large repository within the subarea, while meeting the required respect distances to the deformation zones. This holds true despite a wide range of uncertainty in the geometry of identified deformation zones. There are, however, uncertainties on the suitability of potential deposition volumes north of the Simpevarp peninsula due to lack of data from repository depth in this area. These volumes would be needed, since the space directly below the Simpevarp peninsula is quite restricted.
- Only a few percent of all potential deposition holes would be intersected by discriminating fractures of radius larger than 50 m but the number is uncertain due to the uncertainty in the DFN-model of the fractures.
- A repository can be constructed, at least down to –500 m, without expecting problems with extensive spalling or rock fallout.
- It is possible to define a layout that ensures that the required temperature conditions on canister and buffer are fulfilled.
- The groundwater composition sampled at potential repository depth at the Simpevarp subarea lies well within both the required and preferred bounds. Furthermore, even if the exact spatial distribution of the water composition is uncertain, all the four water types identified also fulfil the hydrogeochemical criteria. This also means that it is likely that the groundwater composition will remain within the range of the criteria also in the future.

The evaluation also shows that the Simpevarp subarea meets *most of the safety preferences*, but for some aspects of the site description further reduction of the uncertainties would enhance the safety case. In particular:

- The thermal conductivity is relatively low and shows rather high and uncertain spatial variability. Unless these uncertainties are reduced, the design would need to consider relatively large canister separations in order to ensure that the temperature requirements on canister and buffer are met.
- Between 60 and 80 percent of blocks at the 20 m scale has an effective hydraulic conductivity $K < 10^{-8}$ m/s. The estimate depends on the conceptual model for the hydraulic discrete fracture network model. This means that there could be some concern as to whether the preference on low hydraulic conductivity is met, especially considering the upper uncertainty bound. However, the preference value for hydraulic conductivity at the canister scale is based on rather simplistic reasoning.
- The evaluation of flow-related transport parameters conducted with the regional groundwater flow model shows that both the preferences for Darcy velocity and the preference for transport resistance F are met for almost all potential migration paths. However, the analysis has not been made with sufficient resolution for a firm conclusion to the drawn, and there are also substantial uncertainties with respect to the channelling of individual fractures.
- The migration properties of the rock matrix (porosity, formation factor and K_d) meet the preferred values. However, the values are based on few samples only.

Consequently, from a safety point of view, there is no reason not to continue the Site Investigations of the Simpevarp subarea. There are still uncertainties to resolve and the safety would eventually need to be verified through a proper safety assessment. Still, this Preliminary Safety Evaluation demonstrates that it is likely that a safe repository for spent nuclear fuel of the KBS-3 type could be constructed at the site.

4.2 Feedback to the continued site characterisation

The Site Descriptive Model report, i.e. SDM S1.2, based on the Initial Site Investigation of the Simpevarp Subarea, /SKB, 2005a/, states that there is uncertainty associated with the description of the Simpevarp subarea. However, the main uncertainties are identified and in some cases quantified, or explored as alternatives.

There are however some uncertainties that remain unquantified at this stage and some alternative hypotheses have not been developed into models. The uncertainty and confidence assessment conducted suggests that the remaining issues for the Simpevarp subarea mainly concern the details at depth of the descriptions of geological, thermal, mechanics, hydrogeological and hydrogeochemical properties. The description of geometry and properties of important deformation zones in the Simpevarp subarea, some of which are repository volume-delineating zones, could ideally also be substantiated by more (borehole) data to assess heterogeneity and provide a statistical description of properties. There are comparatively few data from repository depth on potential repository volumes particularly north of the Simpevarp peninsula (zone ZSMNE012A).

However, this Preliminary Safety Evaluation shows that only some of these quantitative or qualitative uncertainties have safety implications and would need further resolution. The following feedback is provided to the site investigations and the associated site modelling.

- Reducing the uncertainty on the deformation zone geometry within the Simpevarp subarea would allow for a more well defined layout, although the sensitivity analysis shows that the space needed is rather robust with respect to uncertainties in the zones. Nevertheless, acquisition of more data as suggested by SDM S1.2 and subsequent evaluation would be useful.
- There is a need for data from repository depth on potential repository volumes particularly north of the Simpevarp peninsula (zone ZSMNE012A) as these volumes are comparatively less well explored compared with the rest of the Simpevarp subarea. It should also be noted that if the complete site investigation programme was to focus on the Simpevarp subarea, there would be a need for more data in the southern parts of the volume, especially since the suggested repository layout extends outside the current local model domain.
- There is substantial uncertainty in the DFN-model and this affects key safety aspects, like the probability of large fractures intersecting deposition holes, the upscaling of the hydraulic properties and the resulting transport resistance along migration paths from potentially breached canisters. Various alternatives have been presented but it is not clear that these uncertainties span the full uncertainty space. Efforts need to be spent on reducing these uncertainties. During the Site Investigation Phase this can partly be achieved from more data, as further discussed in Chapters 12 and 13 of SDM S1.2, but there is also a limit to the extent to which these uncertainties could be reduced using only surface-based information. Efforts need also be spent on improving the modelling. There are assumptions made in current models that could be challenged and there seems to be room for better use of borehole information. It is especially important to provide robust estimates of the intensity of large fractures and features, e.g. the *k* parameter in the power law distribution, and further efforts should be spent on providing good support for the possible range of this parameter. Observations in the size interval that causes the discriminating fracture intersections, i.e. one to several hundred metres, are scarce. It is therefore desirable to increase the confidence in this interval of the size distributions. In contrast, details of the orientation distribution of fractures are less important.
- The current uncertainty in stress and intact rock properties is sufficiently low for making the safety case. Still, the issue of spalling due to the thermal load may require additional analyses, as already envisaged for SR-Can. This may also lead to additional data demands.
- Even if the thermal requirements and preferences are met, further reduction of uncertainties in the spatial variability and scaling of thermal conductivity would allow for a more efficient design. This could also enhance the safety case, as there would be less strict demands on the layout in order to meet the temperature requirements. Such a reduction could be made through the methods envisaged in Chapter 12 and 13 in SDM S1.2, both as regards measurement and modelling.
- The rather high hydraulic conductivity values observed and the uncertainties in the spatial variation and upscaling warrant further studies. These would concern both additional data, in order to assess potential differences between different rock domains and to better understand potential anisotropy, and additional efforts in evaluating these data. More precise suggestions for how to reduce the uncertainties are given in the SDM S1.2.
- Even if the hydrogeochemical requirements and preferences are met, further reduction of uncertainties would improve the understanding of the hydrogeochemistry and would enhance the safety case. The additional data and evaluations suggested for this in SDM S1.2 are considered justified. SR-Can also intends to carry out a detailed evaluation of the different potential backfill materials and how different salinity levels would affect

them, though not for the Simpevarp sub-area. This evaluation might also result in further needs for a more detailed projection of the present and future salinity distribution at the site.

- In order to evaluate the redox buffering capacity of the geosphere detailed mineralogical data on Fe(II) and sulphide content of the rock and fracture minerals would be needed.
- There is a need to reduce the uncertainty in channelling although this can only partly be achieved by new measurement approaches. Further attention to modelling, with different alternatives and careful scrutiny of assumptions, would elucidate the importance of these uncertainties.
- It is premature, in the PSE, to assess potential data needs for improving the description of the migration properties of the rock matrix – or even whether such improvements would be needed. More *in situ* data would nevertheless improve the safety case.

4.3 Implications for design

The assessments made for the PSE also suggest some implications for design, some of which are of a generic character to be considered also for other sites. The most important such feedback is given below.

Compared with the actual safety requirement, see section 3.2.1, the design rules for discarding canister positions due to potential intersection with large fractures or deformation zones are overly restrictive. The percentage of deposition holes to be discarded would substantially decrease if the design rules were better harmonised with the actual safety requirements.

The spatial variability of the thermal conductivity may be too large for the currently adopted design rules. The additional temperature analyses conducted here suggest that the canister spacing now suggested by design may be insufficient at some canister locations. Increasing the canister spacing would alleviate this problem and it is of course important to carefully select an appropriate spacing since this determines the overall requirements on space for the deep repository.

The temperature margin for gaps and uncertainty/variability in rock thermal conductivity applied in the design work should be revisited, as the present rules seem to leave too little margin for these factors.

4.4 Implications for later safety assessments

Finally, this PSE also highlights issues for attention to be considered if the Simpevarp subarea was to be assessed in a full safety assessment. Most of the issues are rather generic in nature and thus warrant consideration in future safety assessments of other sites.

The percentage of deposition holes intersected by fractures with radius larger than 100 m given in this report does not consider the probability of actually finding such large fractures and thus avoiding disposing waste in unwanted deposition holes. For the Safety Assessment, there is also a need to consider this probability. Preliminary assessments, focusing on finding how precise such practical identification would need to be in order to make the impact of post-glacial faults negligible, will be made in SR-Can.

In stress domain I, but not in stress domain II, there should be some attention to the likelihood and consequences of spalling, due to the thermal load, in deposition holes. However, such spalling is judged unlikely in the Simpevarp subarea, due to the low stress levels.

The relatively high permeability raises some concern although a more useful criterion would be the distribution of Darcy velocity and transport resistance F along potential migration paths. The detailed scale DFN-approach planned for the safety assessment, will alleviate the averaging uncertainties stemming from the porous medium description in the migration analysis discussed in this PSE, but assumptions made on channelling would have an impact on the final numbers.

The actual retention of a radionuclide is element specific and the importance of the retention depends on the release situation and the half-life of the individual radionuclide. The site specific information on the migration properties of the rock needs to be complemented by more generic data and by consideration of how they are affected by the conceptual uncertainties in the migration processes. Combining all such aspects is an important part of a safety assessment and will be done in SR-Can, but lies outside the scope of the PSE.

It seems that the future evolution of the hydrogeochemistry could be sufficiently well bounded by the ranges of the four water types identified in the area. In the safety assessment, it should be assessed whether there could be any process or condition that would invalidate such an assumption.

Finally, there are other site specific issues that need to be considered in a full safety assessment of the Simpevarp subarea. The impact of the existence of Äspö HRL, with its potentially open tunnels, should be considered. There is also a need to assess potential impact on the nuclear power plants and on the interim storage facility for spent nuclear fuel, Clab, from a repository lying directly below these facilities.

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