**Technical Report** 

TR-98-23

# Site-scale groundwater flow modelling of Aberg

Douglas Walker Duke Engineering & Services

Björn Gylling Kemakta Konsult AB

December 1998

#### Svensk Kärnbränslehantering AB

Swedish Nuclear Fuel and Waste Management Co Box 5864 SE-102 40 Stockholm Sweden Tel 08-459 84 00 +46 8 459 84 00 Fax 08-661 57 19 +46 8 661 57 19



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*Keywords:* Canister flux, computer modelling, F-ratio, groundwater flow, Monte Carlo simulation, repository, stochastic continuum, SR 97, travel time

This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

Information on SKB technical reports from1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40), 1990 (TR 90-46), 1991 (TR 91-64), 1992 (TR 92-46), 1993 (TR 93-34), 1994 (TR 94-33), 1995 (TR 95-37) and 1996 (TR 96-25) is available through SKB.

## Abstract

The Swedish Nuclear Fuel and Waste Management Company (SKB) SR 97 study is a comprehensive performance assessment illustrating the results for three hypothetical repositories in Sweden. In support of SR 97, this study examines the hydrogeologic modelling of the hypothetical site called Aberg, which adopts input parameters from the Äspö Hard Rock Laboratory in southern Sweden. This study uses a nested modelling approach, with a deterministic regional model providing boundary conditions to a site-scale stochastic continuum model. The model is run in Monte Carlo fashion to propagate the variability of the hydraulic conductivity to the advective travel paths from representative canister locations. A series of variant cases addresses uncertainties in the inference of parameters and the boundary conditions. The study uses HYDRASTAR, the SKB stochastic continuum groundwater modelling program, to compute the heads, Darcy velocities at each representative canister position and the advective travel times and paths through the geosphere.

The nested modelling approach and the scale dependency of hydraulic conductivity raise a number of questions regarding the regional to site-scale mass balance and the method's self-consistency. The transfer of regional heads via constant head boundaries preserves the regional pattern recharge and discharge in the site-scale model, and the regional to site-scale mass balance is thought to be adequate. The upscaling method appears to be approximately self-consistent with respect to the median performance measures at various grid scales. A series of variant cases indicates that the study results are insensitive to alternative methods on transferring boundary conditions from the regional model to the site-scale model. The flow paths, travel times and simulated heads appear to be consistent with on-site observations and simple scoping calculations.

The variabilities of the performance measures are quite high for the Base Case, but the variability between the studied variants is comparatively low. Variant 4.2, using conditional simulation, yields the shortest median travel time and greatest median canister flux. The anisotropic variogram case, Variant 3.1, yields the longest median travel time and lowest median canister flux. The Base Case results suggest that the expected performance measures of the Aberg hypothetical repository areas are as follows:

- The median travel time is 10 years, with an interquartile range from 3.4 years to 37 years.
- The median canister flux is  $1.8 \times 10^{-3}$  m/year, with an interquartile range from  $3.7 \times 10^{-4}$  m/year to  $7.8 \times 10^{-3}$  m/year.
- The median F-ratio is  $1.0 \times 10^5$  year/m, with an interquartile range from  $3.4 \times 10^4$  year/m to  $3.7 \times 10^5$  year/m.

### Sammanfattning

SR 97 är en säkerhetsanalys av tre hypotetiska djupförvar i Sverige. Denna rapport, utförd som en del av SR 97, beskriver den hydrogeologiska modelleringen av Aberg. Aberg är en hypotetisk plats där indata och parametrar baseras på förhållanden vid Äspölaboratoriet (Äspö Hard Rock Laboratory) som är beläget i södra Sverige. I studien har en nästlad modellering använts där en deterministisk regional modell ger randvillkor till en stokastisk kontinuum modell i platsskala. Monte Carlo simulering har använts för att propagera variabiliteten i hydraulisk konduktivitet till advektiva partikelbanor som utgår från representativa kapselpositioner. I en serie varianter har osäkerheter vid tolkandet av parametrar och överförandet av randvillkor analyserats. För att beräkna tryck, Darcy-hastigheter (specifika flöden) vid kapselpositioner, advektiva gångtider samt partikelbanor genom geosfären har SKB:s stokastiska kontinuumprogram för grundvattenmodellering, HYDRASTAR, använts.

Den hydrauliska konduktivitetens skalberoende samt användandet av en nästlad modelleringsteknik väcker ett antal frågor rörande modellkonsistens samt massbalans mellan regional- och platsskalemodell. Vid överföringen av tidsoberoende tryckrandvillkor från den regionala modellen till platsskalemodellen bevaras mönstren i in- och utsrömningsområden samtidigt som massbalansen mellan modellerna är adekvat. Uppskalningsmetoden för konduktiviteter indikerar konsistenta resultat (i termer av medianvärden på beräknade mätetal) när olika storlekar på modellcellerna har använts. Serien av variationsfall indikerar att resultaten är relativt okänsliga för de alternativa metoder som använts för överföring av randvillkor från regional- till platsskalemodell. Partikelbanor, gångtider och simulerade tryck är i överensstämmelse med observationer gjorda på platsen och med förenklade överslagsberäkningar.

Variabiliteten i de beräknade mätetalen är förhållandevis hög inom basfallet medan skillnaderna mellan variationsfallen är förhållandevis små. Den lägsta medianen för gångtider och den högsta medianen för specifika flöden vid kapselpositioner erhölls för variationsfall 4.2 där konditionering på borrhålsdata använts i simuleringarna. Den högsta medianen för gångtider och den lägsta medianen för specifika flöden vid kapselpositioner erhölls i variationsfall 3.1 som är baserat på ett anisotropiskt variogram. Resultaten för basfallet ger mätetal för förvarsfunktionen i Aberg enligt följande:

- Medianen för gångtiderna är 10 år, med ett spann mellan kvartilerna från 3.4 år till 37 år.
- Medianen för specifikt flöde vid kapselpostioner är  $1.8 \times 10^{-3}$  m/år, med ett spann mellan kvartilerna från  $3.7 \times 10^{-4}$  m/år till  $7.8 \times 10^{-3}$  m/år.
- Medianen för F-faktorn är  $1.0 \times 10^5$  år/m, med ett spann mellan kvartilerna från 3.4  $\times 10^4$  år/m till  $37 \times 10^5$  år/m.

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#### 1 Introduction

#### 1.1 SR 97

Swedish Nuclear Fuel and Waste Management Company (SKB) is responsible for the safe handling and disposal of nuclear wastes in Sweden. This responsibility includes conducting studies into the siting of a deep repository for high-level nuclear waste. The Safety Report 1997 (SR 97) will present a comprehensive performance assessment (PA) of the long-term safety of three hypothetical repositories in Sweden. The PA of each repository will include geosphere modelling to examine the possible transport of radionuclides from the emplaced waste packages through the host rock to the accessible environment. The hypothetical repositories, arbitrarily named Aberg, Beberg and Ceberg, take their data from sites previously investigated by SKB.

#### 1.2 Study Overview

This report presents the site-scale hydrogeologic modelling study of the Aberg hypothetical repository. The Aberg site adopts input parameters from the Äspö Hard Rock Laboratory in southern Sweden, a site previously investigated by SKB. Walker et al. (1997b) summarises the site characterisation studies at Äspö and presents several possible representations for the site hydrogeology. This study applies a nested modelling approach to Aberg, with a deterministic regional model providing boundary conditions to a site-scale stochastic continuum model. The model is run in Monte Carlo fashion to propagate the variability of the hydraulic conductivity to the advective travel paths from representative canister locations. A series of variant cases address uncertainties in the inference of parameters and the boundary conditions.

The study uses HYDRASTAR, the SKB stochastic continuum (SC) groundwater modelling program, to compute the heads, Darcy velocities at each representative canister position, and the advective travel paths through the geosphere. The tasks involved in applying HYDRASTAR to Aberg include the interpretation of the hydrogeologic model into HYDRASTAR format, upscaling of parameters, simulation and sensitivity analysis, interpretation and illustration of results, and summary reporting. The report is organised into the following sections:

Sections 1 and 2 introduce SR 97 and the methods used in this study.

Section 3 describes the hydrogeologic interpretation of the Aberg data, and any adjustments to this data relative to previous reports.

Section 4 presents the Base Case simulation and examines several individual realisations and starting positions in detail.

Section 5 presents the variant case simulations.

Section 6 summarises and discusses the study results.

Appendix A defines the summary statistics.

Appendix B summarises additional regional model calculations specific to this study.

Appendix C presents supplemental calculations for rescaling, geostatistical inference and scoping calculations for travel times.

Appendix D summarises all input parameters used in this report.

Appendix E documents the data sources and data deliveries (e.g., SICADA log files for downloading the borehole data).

Appendix F summarises the additional software used in this study for statistical analysis, error checking and graphical display.

Appendix G presents the HYDRASTAR main input file used for the Base Case simulations in this study.

Appendix H documents the coordinate transforms used in this study and in Munier et al., 1997.

## 2 Modelling Approach

This study uses a stochastic continuum model of the fractured crystalline host rocks to analyse the groundwater flow and advective flow paths. Geostatistical analysis of hydraulic test data is used to infer a model of spatial correlation for the hydraulic conductivity of the site. Geostatistical simulation is used to create hydraulic conductivity fields for a numerical groundwater flow model, which provides groundwater velocities and flow paths from the hypothetical waste canisters (Neuman, 1988). The model is run in Monte Carlo fashion for a large number of simulated hydraulic conductivity fields to create an ensemble of possible flow paths and Darcy groundwater velocity at the representative canister positions (canister fluxes). Separate reports address the subsequent use of these flow paths and fluxes in transport and biosphere modelling.

The site-scale HYDRASTAR model requires a model domain of adequate grid density to represent the known fractures and adequate extent so that the model reflects the regional flow conditions. These conflicting requirements force this study to adopt a nested modelling approach, with the site-scale model taking its boundary conditions from a regional scale model. This permits the site-scale model to use a relatively dense grid while incorporating the regional flow patterns through constant head (Dirichlet) boundaries on the site-scale domain (Ward et al., 1987). The Base Case and several variants examine this nested approach and the resulting flux balances across the site-scale boundaries.

This study uses SKB's Convex 220 computer to run the HYDRASTAR version 1.7.2 code under a strict source code control system. Several additional SKB programs are used for pre- and post-processing of HYDRASTAR input and output. These include INFERENS, a geostatistical analysis and inference program that is used to regularise the variogram of the data to the model scale; TRAZON, which verifies the stream tube starting positions versus the fracture zones; and HYDRAVIS, a graphical post-processor developed from the commercial software package AVS. The commercial software package STATISTICA post-processes and summarises the statistics of HYDRASTAR output. These pre- and post-processing programs are summarised in Appendix F.

#### 2.1 The PA Model Chain

The software tool for the geosphere portion of the safety analysis consists of a chain of PA models, HYDRASTAR – COMP23 – FARF31—BIO42, developed by SKB for use as a computational tool in the 1995 SKB safety analysis project (SR 95). The end product of the PA model chain is the calculation of the probable dose to the biosphere (Figure 2.1-1). This modular approach allows each component of the repository system to be studied separately, with the results combined at the finish to evaluate the performance. The hydrogeologic model, HYDRASTAR, determines the Darcy groundwater velocities at each stream tube starting position (canister flux) and the

advective travel paths through the geosphere. COMP23 is the near-field model, which uses the canister fluxes to determine the release rate for radionuclides from the representative canisters and into the groundwater flow system. FARF31 uses the release rates from the representative canisters and the travel paths through the groundwater flow system to determine the radionuclide flux through the geosphere. BIO42 is the biosphere module, which takes the radionuclide fluxes from the geosphere and determines the dose to potential receptors (SKB, 1996a). Monte Carlo simulations of the PA chain address uncertainty in the input parameters (e.g., hydraulic conductivity, porosity, etc.).

Note that this report presents only the hydrogeologic modelling study, and consequently discusses only the HYDRASTAR portion of the PA model chain.



Figure 2.1-1. SKB PA model chain.

#### 2.2 HYDRASTAR

HYDRASTAR is a stochastic groundwater flow and transport modelling program developed as a quantitative tool for support of the SKB 91 safety analysis project (SKB, 1992). A flow chart summarising the HYDRASTAR algorithm is presented in Figure 2.2-1. The current version, 1.7.2, uses the Turning Bands algorithm (Journel and Huijbregts, 1978) to generate realisations of the hydraulic conductivity field conditioned on the observed hydraulic conductivities. Trends in the data may be included implicitly through the use of ordinary kriging neighbourhoods or prescribed explicitly for specific regions. Hydraulic conductivity measurements at the borehole scale are upscaled to the model calculation scale using a regularisation scheme based on Moye's formula (a corrected arithmetic mean of the packer test hydraulic conductivities within a block; see Norman, 1992a, for details). HYDRASTAR uses the governing equation for either time-dependent or steady state groundwater flow in three dimensions, assuming constant density. The solution to this governing equation is approximated by a node centred finite-difference method to create a linear system of equations. A preconditioned conjugate-gradient algorithm solves the system of equations to arrive at a solution for the hydraulic head at each node. The pilot point inverse method (de Marsily et al., 1984) can be used to calibrate the input hydraulic conductivity field to minimise the error between the simulated and observed hydraulic heads. Transport in the resulting velocity field is modelled as pure advection using a particle tracking scheme.

The process of conditional geostatistical simulation of hydraulic conductivity, calibration via inverse modelling, and particle tracking can be repeated in Monte Carlo fashion to develop empirical probability distributions for the hydraulic conductivity field, and the travel paths and arrival times for advected contaminants (SKB, 1996b).

Starprog AB developed and tested the code under contract to SKB, beginning in 1989 (Norman 1991 and 1992a). Various authors have contributed to the development and testing of the code, most notably Norman (1991 and 1992a), Morris and Cliffe (1994), Lovius and Eriksson (1993, 1994), Walker et al. (1997a) and Walker and Bergman (1998). The test problems include comparisons to well-known analytical and numerical solutions, or are taken from the HYDROCOIN series of test problems (OECD, 1983; Hodgkinson and Barker, 1985). The code also has been applied successfully to the Finnsjön site, as part of the SKB 91 Project (Norman, 1992a and SKB 1992).

This study does not make use of all the available features in the current version of HYDRASTAR. Conditional geostatistical simulation using borehole data is not used, with the exception of Variant 4.2. The Moye's formula upscaling of borehole data is only used as part of INFERENS analysis of the data to infer a variogram model. Trends in the hydraulic conductivity are included as stepwise changes in the geometric mean to represent fracture zones, rock units and decrease with depth (i.e., no continuous decrease with depth is used). The calibration algorithm is not used, nor is the transient simulation of pumping tests.



*Figure 2.2-1. HYDRASTAR version 1.7 flow chart. Superscript "r" denotes realisation number.* 

#### 2.3 Development of Modelled Cases

In addition to data analysis, computer simulation, and post-processing of results, the modelling process also requires that a set of relevant cases be analysed. In practice, expert judgement determines which assumptions to test and which uncertainties to evaluate. The result is a base case that represents the expected site conditions, and several variation cases that assess the uncertainty of inferences and assumptions. For this study, a separate group of scientists was convened by SKB, consisting of:

- Johan Andersson, Golder Grundteknik KB,
- Sven Follin, Golder Golder Grundteknik KB,
- Jan-Olof Selroos, SKB,
- Anders Ström, SKB, and
- Douglas D. Walker, Duke Engineering & Services, Inc.

This group met several times between November 1997 and March 1998, to discuss the reasoning behind the modelling assumptions, the derivation of model parameters and the modelling uncertainties. These discussions resulted in the parameters and assumptions that constitute the Base Case and variant cases addressed in this report.

## 3 Model Application

Walker et al. (1997b) summarises the hydrogeology of the site and proposes a series of parameter sets for use in hydrogeologic modelling. In addition to these preliminary parameter sets, HYDRASTAR also requires a geostatistical description of the hydraulic conductivity that is appropriate for the grid scale of interest. Appendix C presents additional computations for rescaling hydraulic conductivities and the inference of additional geostatistical parameters.

A nested modelling approach is used, with the site-scale model taking its boundary conditions from the much larger regional scale model of Svensson (1997a, and this report, Appendix B). Appendix B summarises the specific regional model simulations used to generate the boundary conditions for the local scale model. The extent of the model domain was evaluated as part of the Alternative Models Project (AMP) of SR 97 (Widén and Walker, 1998) and in preliminary modelling studies (Gylling et al., 1998; Follin, 1998).

The following sections describe the application of HYDRASTAR to the Aberg site, including the hydrogeologic conditions and modelling assumptions.

#### 3.1 Site Description

Aberg takes its data from the Äspö site, which is located in southern Sweden, in the northern part of Småland (Figure 3.1-1). It is just off the Swedish coast in the Baltic Sea, near the Oskarshamn nuclear power plant. The Äspö site is also the location of the Äspö Hard Rock Laboratory (HRL), an underground research facility owned and operated by SKB. From a hydrogeologic perspective, the region is notable for the low topographic relief and the intrusion of saltwater from the Baltic Sea.



Figure 3.1-1. Location of the Äspö site and Hard Rock Laboratory.

### 3.2 Hydrogeology

The geology and hydrogeology of the Äspö site have been studied in great detail and are summarised in a series of reports (Wikberg et al., 1991; Rhén et al., 1997). Walker et al. (1997b), presents a summary of site conditions emphasising continuum modelling.

Äspö regional geology is dominated by fractured crystalline bedrock consisting of the heterogeneous Småland granite suite. The Äspö shear zone running SW-NE through Äspö Island divides the bedrock into two parts. The region continues to experience isostatic rebound as a consequence of the last period of continental glaciation. This glaciation also deposited bouldery till throughout the region. Peatlands are found in some depressions, as are fluvial sand and gravel. The soil cover is thin with numerous bedrock outcrops. Regional lineaments have been mapped and examined by various airphoto, aerogeophysical, outcrop, seismic and borehole studies, revealing a number of major discontinuities that have been interpreted as steeply dipping fracture zones. The salinity profile of the groundwater system is typical of islands and coastal areas: fresh groundwater near the surface rests on saline water that has intruded from the sea.

Hydrogeologic data of the area around and on Äspö were compiled during 1986-1987. Precipitation generally exceeds evapotranspiration, resulting in a small net recharge on the land surface. The classical model of topographic drive suggests that recharge will occur in higher elevations and flow to discharge areas in lower elevations. This should be combined conceptually with the classical model of seawater intrusion under freshwater in coastal areas and islands. Although simplistic, this general model is consistent with the locations of streams, mires, observed hydraulic heads, salinity distributions and geochemical data available in the region. Svensson (1997a, 1997b) used a groundwater flow model to demonstrate that the overall pattern of groundwater flow at depth can be explained by this combination of conceptual models.

#### 3.3 Regional Model and Boundary Conditions

This application of HYDRASTAR uses a nested modelling approach, taking the boundary conditions of the site-scale model from a much larger regional scale model. Svensson (1997a) used a finite difference continuum model, PHOENICS, to study regional flow patterns under various assumptions. Several complementary simulations of the Svensson regional model determined heads and fluxes along the boundaries of the site-scale domain used in this HYDRASTAR application. These complementary simulations were not reported in Svensson (1997a), but are documented in Appendix B. Figure 3.3-1 shows the extent and location of both the regional and site-scale modelling domains.

The model of Svensson (1997a) included the effects of saline Baltic seawater intruding under freshwater. HYDRASTAR cannot simulate density dependent effects, and the discrepancy might result in inappropriate heads being specified along the site model domain. To create boundary conditions more compatible with HYDRASTAR, the Svensson regional model was rerun using freshwater to create boundaries for use in this study. The specifications and the results of that run are summarised in Appendix B of this report. Figure 3.3-2 shows the resulting steady-state head values, which are used as Dirichlet (constant head) boundary conditions by the site model.

Note that the effects of the assumed boundary conditions are evaluated in the boundary condition variant case described in Section 5.1 of this report.

Figure 3.3-1. Äspö site map, showing the Svensson (1997a) regional model (green) and Aberg site-scale model (yellow) (Äspö local coordinate system).



*Figure 3.3-2. Constant head boundary conditions for the Aberg Base Case, on each face of the model domain (freshwater hydraulic head, in metres).* 

The head values pictured in Figure 3.3-2 require some adaptation for use in the smaller scale HYDRASTAR model. The head values generated by the regional model are generated on a 100 m grid spacing, and must be interpolated to the 25 m HYDRASTAR grid spacing. This was accomplished using a MATLAB program for two-dimensional linear interpolation to create a set of head values on each model surface. The output of this MATLAB program was written to a file in the required format for HYDRASTAR as a Dirichlet boundary condition. This process, several alternative methods, and the associated programs are described in Appendices B and F.

This interpolation of heads attempts to match the site-scale boundary heads to the regional scale heads for the same domain (i.e., conservation of energy). Although this approach is the same as used in other nested groundwater models (e.g., Ward et al., 1987), it is also important to verify that the fluxes across the boundary are the same (i.e., conservation of mass). The consistency of the boundary fluxes is discussed further in Section 4.0.

#### 3.4 Model Grid and Repository Layout

The HYDRASTAR model for this application consists of a 3-dimensional finite difference grid with a uniform grid spacing of 25 m. Preliminary modelling studies by Widén and Walker (1998) and Gylling et al. (1998) determined a domain location and extent such that particle paths would not be intercepted by lateral boundaries. Figure 3.4-1 shows the location of the modelled domain, which covers an area of 2400 m by 2200 m and extends to a depth of 1250 m (i.e., approximately 6.3 km<sup>3</sup>). The modelling domain extends slightly farther eastward than that used in Widén and Walker (1998). The resulting grid of 97 x 89 x 49 nodes (width, length and depth, respectively) gives a typical size for HYDRASTAR models that can be run on the SKB CONVEX in the time allotted for this study.

The performance assessment measures are based on travel paths and travel times to exit locations in the accessible environment (i.e., ground surface). Ideally, the model grid upper surface would correspond to the ground surface. This is not possible in this study because HYDRASTAR uses a flat plane for the upper model surface. Consequently the observed ground surface is represented as a horisontal plane with the modelled domain lying below sea level (0 masl). The HYDRASTAR particle tracking algorithm requires a minimum distance of one grid spacing from any model boundary to calculate the velocity vectors, and thus the exit location for these simulations is -25 masl. Depending on the step size for particle tracking, this distance actually varies between -50 to -25 masl with a median of -37 masl in the Base Case. That is, the performance assessment measures are based on exit locations on a horisontal plane at -37 masl.

Figure 3.4-1 also shows the hypothetical repository tunnel layout, a two-level design specified by Munier et al. (1997, tunnel design H). The layout avoids mapped fracture zones, allowing an exclusion zone whose width depends on the fracture zones' classification. The tunnels are placed no closer than 100 m to zones that are classified as certain, and no closer than 50 m to those classified as probable. Note that the tunnel design does not avoid fracture zones classified as possible, such as NNW-2 (see Section

4.5). This study represents the hypothetical waste canisters with 120 locations uniformly scattered over the repository tunnels (Figure 3.4-2). HYDRASTAR uses these 120 representative locations as starting positions for the stream tubes (advective flow paths) and the subsequent travel time, canister flux and F-ratio calculations.



Figure 3.4-1. Äspö island and the Aberg site-scale model domain (blue line). Both repository tunnel levels (-500 and -600 masl) are shown projected to ground surface. (Plan view, Äspö local coordinate system, in metres).

Aberg, -500 m



*Figure 3.4-2a. Aberg hypothetical tunnel layout, upper level (–500 masl). Numbered locations are stream tube starting locations as representative canister positions.* 

Aberg, -600 m



*Figure 3.4-2b. Aberg hypothetical tunnel layout, lower level (–600 masl). Numbered locations are stream tube starting locations as representative canister positions.* 

#### 3.5 Input Parameters

HYDRASTAR's input parameters require a structural, hydraulic, and geostatistical description of the site, all at appropriates scales. This study uses the site-scale description based on measurements taken from the pre-investigation and construction phases summarised in Rhén et al. (1997) and Walker et al. (1997b). Pre-construction investigations and tunnel construction identified a number of fracture zones between 5 to 50 m in width. Fractures elsewhere in the site (i.e., those not included in the deterministic zones) are collectively included in the hydraulic conductivity estimates for the rock mass. Consequently, the modelled domain and the hydraulic conductivity data are divided according to the site structural model (Rhén et al., 1997):

- Rock Domain (RD) relatively unfractured rocks outside the deterministic conductors, whose hydraulic conductivity is inferred from 3 m packer tests in single boreholes. On the site-scale, there are six domains denoted SRD1 through 6.
- Conductor Domain (CD) rocks within the deterministic conductors, whose hydraulic conductivities are inferred from interference tests. On the site-scale, the set of conductors are collectively referred to as SCD.

The principal source of hydraulic conductivity data is the injection and pumping tests performed in the cored boreholes and tunnel probeholes (Figure 3.5-1). The rock domain hydraulic conductivity is inferred from the interpreted hydraulic conductivities of the 3 m packer tests, found in the SKB SICADA database. The SKB geostatistical inference code, INFERENS, is applied to the 3 m tests to infer a variogram for the upscaled hydraulic conductivity of both the rock and conductor domains. The interference tests provide the hydraulic conductivity of the conductor domain (Walker et al., 1997b).

The scale of these measurements (as inferred from the packer length) is much different from the finite difference block scale of the model grid. As discussed in Walker et al. (1997b), hydraulic conductivity is a scale-dependent parameter, requiring that the interpreted hydraulic conductivities be appropriately rescaled for use in the model. That is, we need to determine a block-scale hydraulic conductivity,  $K_b$ , which preserves the expected flux through the domain represented by the block. This study uses the scale dependence of  $log_{10}$  K observed at Äspö to rescale the mean  $log_{10}$  K of block conductivities in a stochastic continuum model. Rhén et al. (1997) and Walker et al. (1997b) provide general analyses of the hydraulic conductivity data and a regression equation describing the Äspö scale dependence. Appendix C.2 of this report summarises the upscaling and inference of parameters for block scales of 25 m, 50 m and the effective conductivity ( $K_e$ ) for the deterministic variant.



Figure 3.5-1. Äspö HRL tunnel and boreholes, from Rhén et al. (1997) (Äspö local coordinate grid).

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#### 3.5.1 Conductor Domain (SCD)

The geometries of the hydraulic conductor domains are defined by the major discontinuities described in Rhén et al. (1997) and represented as planar features of constant width (Figure 3.5-1). This study reduced the effective transmissivities of Rhén et al. (1997) to hydraulic conductivities using the specified widths. The specified width of several of the deterministic structures is less than the model grid spacing of 25 m. This presents a minor problem for HYDRASTAR, whose geostatistical simulation algorithm only includes deterministic features that directly intersect the centres of the block interfaces. Depending on the structure orientation, this might result in anomalous discontinuities in the structure that are solely the result of the grid spacing. To avoid these anomalies, the SCD widths are increased to a minimum width of 25 m and the hydraulic conductivities decreased proportionaly to maintain the transmissivity of the SCD. Note that one deterministic hydraulic conductor, NNW-8, is not shown in Figure 3.5-2 because it is not thought to reach the surface.

Several types of hydraulic tests were performed in the individual conductive structures, including a series of multi-hole interference tests (Rhén et al., 1997). These tests were on varying measurement scales, thought to be between 50 and 100 m (Rhén, personal communication, 1997). This study assumes that these interference tests have a measurement scale of 100 m and rescales the reported hydraulic conductivities using the observed scale dependence at Äspö (Appendix C.2; Table 3-1). As is suggested in Rhén et al. (1997), the median  $\log_{10}$  hydraulic conductivities change by a factor of 1/10 below –600 masl.

Zone	Median Log <sub>10</sub> K (m/s)		Width (m)	Sample size
	100 m	25 m		
EW-1N	-7.3	-7.8	30	4
EW-1S	-6.1	-6.6	30	4
EW-3	-5.8	-6.3	15	4
EW-7	-5.2	-5.7	10	3
NE-1	-5.0	-5.5	30	16
NE-2	-7.1	-7.6	5	12
NE-3	-5.2	-5.7	50	9
NE-4	-6.1	-6.6	40	8
NNW-1	-6.3	-6.7	20	7
NNW-2	-5.6	-6.0	20	4
NNW-3	-6.3	-6.8	20	(ave. of all NNW)
NNW-4	-4.8	-5.3	10	8
NNW-5	-7.0	-7.5	20	3
NNW-6	-6.3	-6.8	20	(ave. of all NNW)
NNW-7	-6.6	-7.1	20	5
NNW-8	-6.3	-6.8	20	3
<b>NW-1</b>	-7.8	-8.3	10	3
SFZ, w	-6.9	-7.4	20	(site data upper
				quartile)
SFZ, ww	-5.4	-5.9	20	(site data lower
				quartile)

Table 3-1. Aberg site-scale conductors (SCD1). 100 m measurements from Rhén et al. (1997), scaled to 25 m. Below –600 masl, all hydraulic conductivities change by a factor of 1/10.


Figure 3.5-2. Aberg site-scale conductor domains (SCD), from Rhén et al. (1997).

### 3.5.2 Site-scale Rock Domain (SRD)

Based on observations during the pre-investigation and construction of the Äspö HRL, the Aberg site is divided into five rock mass domains (SRD) as given by Walker et al. (1997b; see also Figure 3.5-3 in this report). The arithmetic mean of log<sub>10</sub> hydraulic conductivities for domains SRD1-3 is based on the interpreted hydraulic conductivities of the 3 m packer tests. The areas outside the SRDs but inside the model domain are assigned the geometric mean of all the 3 m interpreted hydraulic conductivity. As discussed above, these values must be upscaled from 3 m and 15 m measurement scale to 25 m finite difference grid scale. Table 3-2 presents the upscaled values used in this



Figure 3.5-3. Aberg site-scale rock domains (SRD), from Rhén et al. (1997).

study. The SRDs extend through the entire model depth, with a uniform change in hydraulic conductivity by a factor of 1/10 at -600 masl. This study differs from that of Widén and Walker (1998) in this respect, since the Widén and Walker (1998) model of Aberg had no change below -600 masl.

masl	•	
SRD	Log <sub>10</sub> K (m/s)	
	3 m	25 m
SRD1	-8.7	-8.0
SRD2	-7.8	-7.1
SRD3	-9.5	-8.8
SRD4 *	-7.6*	-7.5
SRD5	-8.3	-7.6
Other (average	-9.3	-8.5
of SRD1 - 3)		

Table 3-2. Hydraulic conductivity for Aberg site-scale rock mass (SRD). 3 m measurements from Rhén et al. (1997), scaled to 25 m. Hydraulic conductivity of all SRD units changes by a factor of 1/10 below –600 masl

Hydraulic properties for SRD4 are somewhat difficult to infer from the data. There are no 3 m tests within SRD4 (southern Äspö, south of NE-1); consequently, the interpreted hydraulic tests in the tunnel probeholes are used to infer hydraulic properties for SRD4. These probehole tests were conducted and interpreted in a different manner from the 3 m tests in the cored boreholes, leaving a suspected bias (Rhén, personal communication, 1997). Svensson (1997a) evaluated the conductivity of SRD4 via inverse modelling of the drawdowns of hydraulic heads induced by the excavation of the HRL. Svensson found that reducing the hydraulic conductivity of SRD4 by approximately one order of magnitude improved the agreement between modelpredicted and observed drawdowns. This study uses Svensson's calibrated value of mean log<sub>10</sub> hydraulic conductivity for SRD4, with adjustments for scale (Table 3-2).

#### 3.5.3 Geostatistical Model

The Aberg site-scale geostatistical model of hydraulic conductivity consists of the rock blocks described for SRD1 through 5, the SCD and a single variogram model. As is discussed in Walker et al. (1997b), the variogram must be adjusted (regularised) to account for the difference between measurement and grid scales. Note that only one variogram model can be specified in HYDRASTAR for both domains. Because the experimental variogram of the 3 m data in the conductors is erratic, this study infers a regularised variogram model based on the upscaled 3 m packer test data in the rock domain for both the SRD and SCD (Walker et al., 1997b). Unlike previous geostatistical studies of the Äspö data (La Pointe, 1994; Winberg, 1994; Niemi, 1995), this study uses the interpreted hydraulic conductivities of Rhén et al. (1997) for the 3 m packer tests. This is important because the Rhén interpretation has no lower measurement limit, a characteristic that can effect the statistics of the data. The interpreted conductivities are taken from cored boreholes KLX01, KAS02, KAS03, KAS04, KAS05, KAS06, KAS07 and KAS08, as found in SICADA. The SKB code INFERENS was used to upscale the 3 m data to 25 m and fit a model variogram and trends to the upscaled data (Walker et al., 1997b).

Results of this analysis indicated the following variogram model for the 25 m grid scale (Figure 3.5-4):

- Exponential model, isotropic,
- Practical range of 97 m, and
- Zero nugget,  $\log_{10}$  K variance 2.72.

The SRD and SCD are treated as step changes in the logarithm of block conductivities (i.e., 0 order trends in arithmetic mean of  $log_{10} K_b$ ), with values provided in Tables 3-1 and 3-2. Figure 3.5-5 shows the HYDRASTAR representation of the SCD, and Figures 3.5-6 and 3.5-7 show the combination of the SCD and SRD via a plot of the deterministic  $log_{10} K_e$  field. The combined effects of this geostatistical model of Aberg are illustrated in Figure 3.5-8, which presents a single realisation of the Base Case hydraulic conductivity field.



Figure 3.5-4. Semivariogram of  $log_{10}$  of hydraulic conductivity for Aberg rock domain. 3 m data in rock domain, upscaled to 25 m and fitted via INFERENS.



*Figure 3.5-5. HYDRASTAR representation of Aberg conductive fracture zones (SCD). (Isometric view from southwest and slightly above).* 

The Base Case geostatistical model represents the rock domains and conductive fracture zones deterministically, extending throughout the entire depth of the model (Figures 3.5-2 and 3.5-3, respectively). This deterministic representation is used even though the occurrence and extent of the SCD and SRD are uncertain and additional, undetected structures are possible (Rhén et al., 1997). An alternative HYDRASTAR option is available that includes large-scale structures stochastically via conditional geostatistical simulation (i.e., conditioning the fields using the measured hydraulic conductivity data). This latter approach tends to create structures whose size is limited by the data density of the range of the variogram. For the Aberg site, the inferred range is relatively short and the data is widely spaced, so that this conditional simulation approach generally will not create fields with conductive zones as extensive as those suggested by Rhén et al. (1997). Consequently, the Base Case geostatistical model uses a deterministic SCD and evaluates the associated uncertainty with a variant case for conditional simulation (Variant 4). This uncertainty does suggest an enhancement of the current version of HYDRASTAR to include a geostatistical simulation method that addresses large-scale structures stochastically (e.g., Indicator Categorical simulation).



Figure 3.5-6. Log<sub>10</sub> of hydraulic conductivity on the upper model surface in Aberg. Variant 5 (deterministic representation of hydraulic conductivity, Äspö local coordinate system, scale in metres).



*Figure 3.5-7.* Log<sub>10</sub> of hydraulic conductivity in Aberg Variant 5 (deterministic representation of hydraulic conductivity) on a plane cutting through the upper repository level (Äspö local coordinate system, scale in metres).





Figure 3.5-8. One realisation of  $log_{10}$  of hydraulic conductivity for the Aberg Base Case in a) plan view at z = 0 masl and b) on the southern model surface. (Äspö local coordinate system, scale in metres).

### 3.5.4 Other Parameters

The remaining HYDRASTAR input parameters are hydraulic parameters required for the advective transport calculations and performance measures. One of these is the flow (or kinematic) porosity,  $\varepsilon_f$ , which is generally acknowledged to be an uncertain parameter. Based on the site-specific data of Rhén et al. (1997), this study uses a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ , uniform over the entire domain. It should be noted that the travel times reported in this study are directly proportional to this assumed flow porosity.

Another uncertain parameter is  $a_r$ , the flow-wetted surface area per rock volume. Similar to the flow porosity, the flow-wetted surface is assumed to be uniform over the entire model. As part of studies in support of SR 97, Andersson and Stigsson (1999) analysed the conductive fracture frequency at Äspö and recommended a flow-wetted surface of  $a_r = 1.0 \text{ m}^{-1}$ . This parameter is not used directly as model input for HYDRASTAR, but it is used in calculating the F-ratio, defined as:

$$F = \frac{d_w a_r}{q_w} = \frac{t_w a_r}{\varepsilon_f}$$

Where:

$$\begin{split} &d_w = \text{travel distance for a particle [metres]} \\ &q_w = \text{Darcy velocity} = \ v \cdot \epsilon_f \ [\text{metres/year}] \\ &a_r = \text{specific surface per rock volume for a travel path [m<sup>-1</sup>]} \\ &\epsilon_f = \text{flow (kinematic) porosity [ . ]} \end{split}$$

The F-ratio [years / m] is a ratio of resisting to driving forces for transport, which has been used to compare model results in performance assessments (SKI, 1997). Although the F-ratio is calculated for all cases, it is a simple multiple of the travel time and is therefore plotted only for the Base Case. SR 97 uses the F-ratio to compare the geosphere performance for the three hypothetical repositories, where the flow-wetted surface varies from site to site.

# 4 Base Case

This section of the report presents the Base Case simulation and analysis. The Base Case represents the expected site conditions as described in the Section 3.0, and it is the reference case for comparison to all other cases. The premodelling study of Gylling et al. (1998) examined the extent of the domain and suggested a volume likely to contain all exit locations. Boundaries for this domain are specified head (Dirichlet) boundaries on all sides of the model domain, taken from the steady-state head values of a deterministic, freshwater simulation of the regional model. The details of the regional simulation and boundary condition transfer are given in Appendix B. The hydraulic conductivity field is created via unconditional simulation (i.e., no direct use of measured hydraulic conductivities), prescribing the mean of  $log_{10}K$  for each rock unit (SRD and SCD).

100 realisations of the hydraulic conductivity field, each with 120 starting locations, are used to estimate the distributions of travel time and canister fluxes. All statistics are calculated with respect to the common logarithm transform ( $log_{10}$ ) of the travel times, canister fluxes, and F-ratios to facilitate summary and display.

# 4.1 Monte Carlo Stability

A practical consideration in Monte Carlo simulation studies is that statistics of interest for the model results be stable with respect to the number of realisations. That is, the number of realisations is adequate for reliable estimates of the variability of the results. This study monitored the stability of the estimators of the median travel time and median canister fluxes to stable with respect to the number of realisations. Figures 4.1-1 and 4.1-2 present the medians of the logarithm of travel time and the logarithm of canister flux, respectively, versus the number of realisations. The plots indicate these statistics are approximately constant after 30 realisations, with less than 3 % deviation from the median travel time or median canister flux for additional realisations. This suggests that for the purposes of this study, a total number of 100 realisations are adequate for estimating the medians of the performance measures.

The stability of the sample median should not be taken to imply that higher moments such as the sample variance are also stable. Estimators of higher moments and the extreme quantiles of distributions are usually much less efficient than the median or the mean (Larsen and Marx, 1986). In general, estimating these moments with a similar degree of accuracy requires many more realisations than are needed for stable estimators of the median (Hammersley and Handscomb, 1975). Consequently, the higher-order statistics may not have stabilised and should be used cautiously.



Figure 4.1-1. Monte Carlo stability in the Aberg Base Case. Median travel time versus number of realisations. Results for a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and travel times less than 10,000 years.



Figure 4.1-2. Monte Carlo stability in the Aberg Base Case. Median canister flux versus number of realisations.

### 4.2 Boundary Flux Consistency

Stochastic continuum theory suggests that, under certain conditions, there exists an effective hydraulic conductivity,  $K_e$ , that satisfies:

$$\left\langle \vec{q} \right\rangle = -K_e \nabla \left\langle \vec{h} \right\rangle$$

Where:

 $\langle \bar{q} \rangle$  = the expected flux over the domain

 $\nabla \langle \vec{h} \rangle$  = the expected gradient.

 $K_e$  is useful for nested models in that it can be used to estimate the expected value of the flux in a smaller domain (Dagan, 1986; Rubin and Gómez-Hernández, 1990). This suggests that a regional model with a homogeneous hydraulic conductivity of  $K_e$  could be used to determine the expected boundary fluxes of a site-scale model subdomain. If the rescaling of the geometric mean hydraulic conductivity is correct, the boundary flux of the regional model should be consistent with the average boundary flux of the site-scale stochastic continuum model. That is, the site-scale stochastic continuum model should conserve mass in an average sense with respect to the regional model fluxes.

Walker et al. (1997b) suggested that the upscaling of block scale hydraulic conductivity could be calibrated using the above relationship, adjusting the block scale mean until the average boundary fluxes of the ensemble matched the regional scale fluxes. However, there are several drawbacks to that approach. For example, the existence of  $K_e$  requires that the domain be stationary (statistically homogeneous), a condition that may be violated by the fracture zones interrupting the Aberg host rocks. Although the individual rock blocks (such as the SRDs) may be stationary,  $K_e$  also requires that the domain be extensive and under uniform flow conditions. In addition, although the regional models may conserve mass balance over the entire domain, they do so in an average sense. Consequently, the regional model may not conserve mass for the small subdomain corresponding to the site scale model of interest. This study reports and compares the boundary fluxes, but does not adjust the mean block hydraulic conductivity.

The regional model of Svensson (1997a) used a single stochastic realisation of heterogeneous hydraulic conductivities, with density-dependent flow effects of saline groundwater. For base case of this study, the Svensson regional model was rerun using homogeneous hydraulic conductivity of  $K_e$  and nonsaline conditions to determine the expected boundary heads and fluxes for the Base Case of the site scale model. Appendix B summarises the details of this regional simulation and its results. Variant 1 addresses the consequences of using other regional models and boundary transfer algorithms, in Section 5.1 of this report. Lovius (1998) describes the computation of boundary fluxes for a HYDRASTAR model domain, yielding the average flux over each boundary.





Figure 4.2-1 and Table 4-1 present the boundary fluxes for the Base Case model in comparison to the regional model (Appendix B). As shown in Figure 4.2-1, both models indicate that the majority of the inflow to the domain comes from the west, and the majority of the outflow is directed out the upper surface of the model to the Baltic Sea. This is consistent with the regional pattern of recharge and discharge. Table 4-1 summarises the boundary fluxes as the net flux over each face of the subdomain. The average of 5 realisations of the site model suggested that the site model tends to underestimate the regional boundary fluxes by a factor of approximately 1/2. It may be possible to adjust the mean of  $\log_{10}$  hydraulic conductivities in an attempt to match the boundary fluxes, but this study has not attempted to do so.

Net Flux Through Site Model Surf (m <sup>3</sup> /s x 10 <sup>-3</sup> )		
Site Model Surface	Regional Model (Appendix B)	Site-Scale Model (5 realisations)
West	13.7 (in)	4.92 (in)
East	0.916 (in)	0.77 (in)
South	1.81 (in)	0.846 (in)
North	0.625 (in)	0.538 (in)
Bottom	0.374 (in)	1.03 (in)
Тор	18.1 (out)	8.11 (out)
Total Inflow	17.4	8.10
Total Outflow	18.1	8.11
Mass balance (In-Out)	-0.675	-0.00681

 Table 4-1. Boundary flux consistency for Aberg Base Case, regional model versus site-scale model.

# 4.3 Ensemble Results

### 4.3.1 Travel Time and F-ratio

In each realisation, HYDRASTAR calculates the travel times for a particle to be advected from each starting position (release position) to the model surface. The resulting stream tubes are used later in one-dimensional transport calculations in the PA model chain. Although the advective travel time is a common statistic for comparing variant simulations, it is important to note that HYDRASTAR allows only a homogenous flow porosity to be specified for the entire domain. Consequently, the travel time in any stream tube is directly proportional to this homogeneous flow porosity. This study simply uses the flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ , and leaves further analysis of the flow porosity to the transport modelling studies associated with SR 97.

Figure 4.3-1 presents the frequency histogram of the common logarithm of travel time for 100 realisations. Each of these realisations has 120 starting positions as representative canister locations. A few outliers are seen at the upper tail of the histogram, corresponding to travel times of 10,000 years. These 0.4833 % are stream tubes that are intercepted by the side boundaries and fail to exit the upper surface of the model (Figure 4.4-1). In this circumstance, HYDRASTAR sets the travel times for these stream tubes to the default maximum travel time of 10,000 years.

The use of the default travel time does have noticeable effects on the performance measure statistics, as shown in Table 4-2 for the Base Case. To evaluate this effect, this study calculates the statistics both with and without the travel times greater than 10,000 years. The means and variances of the travel time and F-ratio change slightly if stream tubes with the default travel time of 10,000 years are deleted. In contrast, the canister flux statistics are virtually unaffected by this censoring, as are the medians of travel time and F-ratio. For the remainder of this study, the performance measure statistics are calculated both with and without the travel times greater than 10,000 years. For the sake of brevity, the discussions will emphasise the medians of all measures and the statistics of travel time and F-ratio for travel times less than 10,000 years. The canister flux will be summarised with statistics computed for the full set of stream tubes (no deletions). The variances and medians of the performance measures are emphasised in bold in the summary tables (e.g., Table 4-2). The effects of this censoring on subsequent performance assessment calculations are beyond the scope of this study.

Table 4-2 summarises the ensemble results, presenting the statistics for the 100 Monte Carlo realisations of the 120 starting positions for travel time, as well as canister fluxes and F-ratio. With the intercepted stream tubes deleted, the median of the travel time is 10 years, with an interquartile range from 3.4 years to 37 years.



Figure 4.3-1. Relative frequency histogram of  $log_{10}$  travel time for the Aberg Base Case. Results for 100 realisations of 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .

Table 4-2.	Summary statistics for Aberg Base Case. Results for 100 realisations of
	120 starting positions, a flow porosity of $\varepsilon_f = 1 \times 10^{-4}$ and flow-wetted
	surface $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.

	All values		Travel Times > 10,000 years				
					deleted		
	$\mathbf{Log}_{10}$	$\mathbf{Log}_{10}  \mathbf{q_c}$	$\mathbf{Log}_{10} \mathbf{F}$ -	$\mathbf{Log}_{10} \mathbf{t}_{\mathbf{w}}$	$\mathbf{Log}_{10} \ \mathbf{q_c}$	$\mathbf{Log}_{10} \mathbf{F}$ -	
	t <sub>w</sub>		ratio			ratio	
Mean	1.083	-2.799	5.083	1.069	-2.796	5.069	
Median	1.021	-2.736	5.021	1.015	-2.734	5.015	
Variance	0.637	0.935	0.637	0.599	0.931	0.599	
5 <sup>th</sup> percentile	-0.125	-4.479	3.875	-0.125	-4.475	3.875	
25 <sup>th</sup> percentile	0.534	-3.430	4.534	0.533	-3.427	4.533	
75 <sup>th</sup> percentile	1.574	-2.114	5.574	1.563	-2.113	5.563	
95 <sup>th</sup> percentile	2.468	-1.298	6.468	2.431	-1.298	6.431	

Figure 4.3-2 shows the frequency histogram of the common logarithm of F-ratio for 100 realisations for travel times less than 10,000 years. This histogram is essentially identical to the histogram of  $log_{10}$  travel times (Figure 4.3-1) because the F-ratio is a simple multiple of the travel time (see Section 3.5.4). This report presents the F-ratio for

all variants, but in the interest of brevity will present the histogram of F-ratio only for the Base Case.

Figure 4.3-3 presents a box plot of the simulated travel times by realisation, which show a wide range of variability. Figure 4.3-4 presents the number of realisations with travel times less than 1 year and 10,000 years, by stream tube number. Because each stream tube number corresponds to a particular starting position, this plot also suggests that some positions tend to have shorter travel times (See Figures 3-5a and b). For example, starting positions 13 through 19, 41 through 50, 74 through 81, and 99 through 120 lie in rock blocks SRD2 and SRD4. These blocks have mean log<sub>10</sub> hydraulic conductivities that are higher then the remaining host rocks. Consequently, stream tubes with starting positions in SRD2 and SRD4 have reduced travel times. Individual starting positions are discussed in greater detail in Section 4.5, and the results by repository level are discussed in Section 4.6.



Figure 4.3-2. Relative frequency histogram of  $log_{10}$  F-ratio for the Aberg Base Case. Results for 100 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1x10^{-4}$  and  $a_r = 1.0 \text{ m}^{-1}$ .



*Figure 4.3-3. Travel times by realisation for the Aberg Base Case. Results for flow* porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



Figure 4.3-4. Number of realisations with travel times less than 1 year (squares) and 10,000 years (lines), by stream tube number for the Aberg Base Case. Results for flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .

### 4.3.2 Canister Flux

HYDRASTAR calculated the canister fluxes (Darcy groundwater velocity) at each of the 120 stream tube starting positions. Table 4-2 summarises the results for the canister flux, which indicate a median canister flux of  $1.9 \times 10^{-3}$  m/year and an interquartile range from  $3.7 \times 10^{-4}$  m/year to  $7.8 \times 10^{-3}$  m/year. Figure 4.3-5 presents the frequency histogram for the log<sub>10</sub> canister flux for 100 realisations, each with 120 starting positions. Similar to the histogram of log<sub>10</sub> travel time, this histogram is also slightly skewed, but in opposite direction. Figure 4.3-6 confirms that the logarithm of travel time is inversely correlated to the logarithm of canister flux. This might not be true for models that use a spatially variable porosity, rather than a homogeneous porosity as is used in HYDRASTAR. Figure 4.3-7 presents a box plot of canister fluxes by realisation, which indicates a variability of over 3 orders of magnitude.



*Figure 4.3-5. Relative frequency histogram of log*<sub>10</sub> *canister flux for the Aberg Base Case. Results for 100 realisations, each with 120 starting positions.* 



Figure 4.3-6.  $Log_{10}$  travel time versus  $log_{10}$  canister flux for the Aberg Base Case. Results for 100 realisations of 120 starting positions and a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .



*Figure 4.3-7.* Box plot of log<sub>10</sub> canister flux by realisation number for the Aberg Base Case. Results for 120 starting positions.

### 4.3.3 Exit Locations

HYDRASTAR calculates the exit locations for each of the particles as the last point of the travel path. Figure 4.3-8 presents a map of the exit locations on the model surface (-25 masl). As discussed earlier in this section, the flow paths are predominantly upward, reflecting the pattern of regional upward groundwater flow. The flow paths are also directed southward to exit locations in the shallow waterways just south of Äspö Island, reflecting the pattern of precipitation recharge on the island, discharging to the surrounding Baltic Sea. The exceptions to this pattern are the flow paths from the starting positions in the northeastern areas of the repository, which are influenced by the recharge under Mjälen.



Figure 4.3-8. Exit locations for the Aberg Base Case. Repository tunnels at –500 masl are shown as projected up to the model surface. Results for 100 realisations of 120 starting positions. (Äspö local coordinate system, scale in metres).

### 4.3.4 Validity of Results

An approximate calculation of the travel time from SRD 1 was performed as a check on the validity of the model (Appendix C.3). These computations used Darcy's law, the estimated gradient, a simple flow path, and the mean hydraulic conductivities to

estimate the advective travel time. The results showed that the travel times should be on the order of 10 years, roughly in agreement with the median of the model results.

In a previous study of the Äspö site, Svensson (1997b, cited in Rhén et al., 1997) determined the advective travel times from -450 masl to ground surface. Using a nonuniform flow porosity with an average of  $\varepsilon_f = 4 \times 10^{-3}$ , Svensson found that 15% of the particles would have reached the surface after 100 years. Although Svensson's model used a spatially variable flow porosity, the results can be roughly rescaled to a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  by dividing the travel times by 40 (i.e., 15% of the stream tubes would have arrived at ground surface after 2.5 years). This suggests that the travel times of this study are roughly comparable to those of Svensson (1997b).

It is also useful to compare the observed heads from boreholes at Äspö model simulated heads. Rhén and Forsmark (1993) provide a suitable set of observations to use for this comparison, the preconstruction undisturbed freshwater heads, estimated as a long term average of the transient heads in open boreholes and packed-off sections at the site. Figure 4.3-9 presents the Base Case simulated versus observed heads at locations corresponding to representative borehole sections at the site. These sections are:

- HAS02 (MA27) is north of EW-1, above 100 m;
- KAS03 (MA32) is north of EW-1, below 100 m;
- HAS13 (MA137) is south of EW-1, above 100 m;
- KAS06 (MA63) is south of EW-1, below 100 m; and
- KAS06 (MA65) is south of EW-1, in zone EW-3.

Because this is a Monte Carlo study of heterogeneous fields, each realisation will not exactly match the observed data. Based on a simple analysis of the errors (Appendix C.4), the maximum error of observed versus model simulated heads should be approximately 2.0 m. The heads of five realisations presented in Figure 4.3-9 are generally within this error, suggesting that the model-simulated heads agree with the observed heads.



Figure 4.3-9. Observed and simulated freshwater heads for five realisations of the Aberg Base Case.

# 4.4 Individual Realisations

There are several strategies that could be used to select several realisations that are in some sense representative of the ensemble. For example, we could select a realisation whose travel time or canister flux is close to the median of the ensemble of the realisations. However, the probability of each realisation in a Monte Carlo set is equal by definition, so that no single realisation can be said to be representative of the ensemble. To illustrate the variability within and between realisations, this study examines three random realisations to get a sense of the ensemble behaviour. (Note that these are actually the first three realisations, whose sequence is randomised by the random number generation).

Figure 4.4-1 presents the stream tubes for realisation number one in plan and elevation views. The stream tubes reflect the overall upward flow pattern at the site, as a result of the regional discharge. The precipitation recharge on the land surface diverts the stream tubes around the islands to discharge areas under the Baltic. As discussed in the previous sections, this flow pattern is a consequence of the regional flow pattern and the effect of the island hydrology. The exit locations of the ensemble are discussed in Section 4.1.5. Figure 4.4-2 presents the stream tubes for realisations 1 through 3, showing the variability of stream tubes and exit locations between realisations. For the first three realisations, Figure 4.4-3 presents the histograms of travel time, canister flux and F-ratio, and Table 4-3 presents the summary statistics. Note that, although the stream tubes and exit locations can vary widely between realisations, the median travel

times and median canister fluxes are rather stable. This is further illustrated in Figures 4.4-4 and 4.4-5, which present plots of travel time and canister flux by starting position number for these three realisations. These plots also show that in any given realisation, the results for a particular starting position can vary widely. Section 4.5 discusses the results for individual starting positions of interest in greater detail.



a) Plan view



b) Elevation view, from South



tw = Ground water travel time (years)

c) Elevation view, from East

Figure 4.4-1. Stream tubes for Aberg Base Case realisation number 1. The y-positive axis of a) points in the direction of Aspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



Figure 4.4-2. Stream tubes for 3 realisations of the Aberg Base Case. Plan view with the y-positive axis pointing in the direction of Äspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



Figure 4.4-3. Realisations 1, 2 and 3 of the Aberg Base Case, statistics taken over all starting positions. Floating histograms of a) log10 travel time, b) log<sub>10</sub> canister flux. Results for a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

$\frac{1}{1000} \text{ surface } a_r = 1.0 \text{ m}/\text{m}^2. \text{ St}$	atistics in dold a	re alscussea in	iext.
	<b>Realisation 1</b>	<b>Realisation 2</b>	<b>Realisation 3</b>
Log <sub>10</sub> Travel Time for times <			
10,000 years (years)			
Mean	0.992	1.000	1.034
Median	0.875	0.966	0.975
Variance	0.578	0.636	0.501
5 <sup>th</sup> percentile	-0.172	-0.399	-0.164
25 <sup>th</sup> percentile	0.477	0.450	0.565
75 <sup>th</sup> percentile	1.410	1.525	1.511
95 <sup>th</sup> percentile	2.454	2.466	2.230
Log <sub>10</sub> Canister Flux for all times			
(m/year)			
Mean	-2.745	-2.699	-2.842
Median	-2.667	-2.558	-2.702
Variance	0.735	0.949	0.818
5 <sup>th</sup> percentile	-4.127	-4.279	-4.506
25 <sup>th</sup> percentile	-3.438	-3.405	-3.507
75 <sup>th</sup> percentile	-2.095	-1.999	-2.175
95 <sup>th</sup> percentile	-1.467	-1.467	-1.528
Log <sub>10</sub> F-ratio for times < 10,000			
years (year/m)			
Mean	4.992	5.000	5.034
Median	4.875	4.966	4.975
Variance	0.578	0.636	0.501
5 <sup>th</sup> percentile	3.828	3.601	3.836
25 <sup>th</sup> percentile	4.477	4.450	4.565
75 <sup>th</sup> percentile	5.410	5.525	5.511
95 <sup>th</sup> percentile	6.454	6.466	6.230
Percent of Stream tubes Failing to Exit	0	0.833	0.833

Table 4-3. Summary statistics for three realisations of Aberg Base Case. Results for 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.



Figure 4.4-4. Log<sub>10</sub> travel time by stream tube number for 3 realisations of the Aberg Base Case. Results for a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .



*Figure 4.4-5.* Log<sub>10</sub> canister flux by stream tube number for 3 realisations of the Aberg Base Case.

# 4.5 Individual Starting Positions

This study examines three individual stream tube starting positions to illustrate the performance of specific repository areas:

- Position 28, in the upper repository level that lies in rock unit SRD3 (rock block with relatively low conductivity, in the central part of the repository) with moderate travel times;
- Position 32, in the upper repository level that lies in rock unit SRD3. This position lies in NNW-2, a fracture zone whose occurrence is thought to be possible but is not well-defined (Munier et al, 1997; Rhén et al., 1997); and
- Position 51, in the upper repository level that lies in rock unit SRD4 (rock block with relatively high conductivity, in the southern part of the repository) with relatively short travel times.

Table 4-4 presents the summary statistics for the three starting positions listed above, compiled over all 100 realisations of the Base Case. As expected, the canister flux of starting position 32 is the highest of the three as a result of being within fracture zone NNW-2. Similarly, the canister fluxes of starting positions 51 and 28 are higher and lower, respectively, than the median canister flux of the entire ensemble (Table 4-4). The histograms of Figures 4.5-1 and 4.5-2 illustrate the relative performance of these starting positions, and also show that the differences are less dramatic for the travel times than the canister fluxes. Figure 4.5-3 is a plot of log<sub>10</sub> travel time versus realisation number for these three starting positions, which shows that the travel time for any given starting position can vary by 3 orders of magnitude between realisations.

	St	arting Position Num	lber
Log <sub>10</sub> Travel Time for times < 10,000 years	28	32	51
(years)			
Mean	1.487	0.497	0.656
Median	1.478	0.420	0.554
Variance	0.384	0.349	0.497
5 <sup>th</sup> percentile	0.459	-0.369	-0.435
25 <sup>th</sup> percentile	1.078	0.125	0.190
75 <sup>th</sup> percentile	1.869	0.886	1.132
95 <sup>th</sup> percentile	2.555	1.498	1.883
Log <sub>10</sub> Canister Flux			
for all times (m/year)			
Mean	-3.111	-1.863	-2.428
Median	-3.061	-1.725	-2.352
Variance	0.727	0.516	0.824
5 <sup>th</sup> percentile	-4.519	-3.218	-3.988
25 <sup>th</sup> percentile	-3.742	-2.211	-3.006
75 <sup>th</sup> percentile	-2.480	-1.376	-1.731
95 <sup>th</sup> percentile	-1.949	-0.844	-0.996
Log <sub>10</sub> F-ratio for times			
< 10,000 years			
(year/m)			
Mean	5.487	4.497	4.656
Median	5.478	4.420	4.554
Variance	0.384	0.349	0.497
5 <sup>th</sup> percentile	4.459	3.631	3.565
25 <sup>th</sup> percentile	5.078	4.125	4.190
75 <sup>th</sup> percentile	5.869	4.886	5.132
95 <sup>th</sup> percentile	6.555	5.498	5.883

Table 4-4.	Summary statistics for three starting positions in the Aberg Base Case.
	Results for 100 realisations, a flow porosity of $\varepsilon_f = 1 \times 10^{-4}$ and flow-
	wetted surface $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.



Figure 4.5-1. Floating histogram of  $log_{10}$  travel time for three starting positions in the Aberg Base Case. Results are for 100 realisations and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



Figure 4.5-2. Floating histogram of  $log_{10}$  canister flux for three starting positions in the Aberg Base Case. Results for 100 realisations.



Figure 4.5-3. Log<sub>10</sub> travel time versus realisation number for three starting positions in the Aberg Base Case. Results for 100 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

As was discussed in Section 4.1, it is important to examine the Monte Carlo stability of the estimators of the statistics of interest. Figure 4.5-4 presents the accumulated median of  $log_{10}$  travel time versus the number of realisations for each of the starting positions discussed above. The median  $log_{10}$  travel time for an individual starting position apparently requires more realisations to stabilise than the ensemble of starting positions, and may not have stabilised at all for position 32 (located within NNW-2). This suggests that evaluating the performance of individual positions may require more realisations than does the performance of the entire repository. Figure 4.5-5 presents the stream tubes for each of theses starting positions, showing that the exit locations can vary by as much as a kilometre.



Figure 4.5-4. Monte Carlo stability at starting positions 28, 32 and 51 in the Aberg Base Case. Median log travel time versus number of realisations. Results for a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



Figure 4.5-5. Stream tubes for Aberg Base Case, a) starting position 28, b) starting position 32, and c) starting position 51. Plan view with the y-positive axis pointing in the direction of Äspö local North. Results for a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

# 4.6 Repository Level

As discussed in Section 3.4, the Aberg repository design is divided into two levels of tunnels, an upper level at -500 masl and a lower level at -600 masl. This study represents the waste canisters by scattering 120 stream tube starting positions uniformly over both levels of the hypothetical repository. This section of the report examines the ensemble results of the Base Case to see if any differences can be observed in the performance of the repository by level.

Figures 4.6-1 and 4.6-2 present histograms for the Base Case, sorted by repository level, of the  $log_{10}$  travel time and  $log_{10}$  canister flux, respectively. The summary statistics for each level are presented in Table 4-5. Although the distributions of travel time and canister flux are very similar, the canister fluxes of the lower repository level are lower and the travel times are slightly greater than that of the upper level. The canister fluxes are lower because of the reduced hydraulic conductivity in the model domain below -600 masl (Section 3.5.3). The travel times of the lower level are longer as a consequence of both the reduced canister flux and the additional 100 m travel distance.



Figure 4.6-1. Floating histogram of  $log_{10}$  travel time by repository level for the Aberg Base Case. Results for 100 realisations of 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



*Figure 4.6-2. Floating histogram of*  $log_{10}$  *canister flux by level for the Aberg Base Case.*
discussed in te	ext.		
	Repository Level		
Log <sub>10</sub> Travel Time for	-500 masl	-600 masl	
times < 10,000 years			
(years)			
Mean	1.035	1.103	
Median	0.989	1.039	
Variance	0.619	0.576	
5 <sup>th</sup> percentile	-0.187	-0.051	
25 <sup>th</sup> percentile	0.489	0.569	
75 <sup>th</sup> percentile	1.536	1.592	
95 <sup>th</sup> percentile	2.383	2.451	
Log <sub>10</sub> Canister Flux			
for all times (m/year)			
Mean	-2.736	-2.862	
Median	-2.676	-2.794	
Variance	0.918	0.944	
5 <sup>th</sup> percentile	-4.393	-4.568	
25 <sup>th</sup> percentile	-3.356	-3.494	
75 <sup>th</sup> percentile	-2.058	-2.174	
95 <sup>th</sup> percentile	-1.267	-1.357	
Log <sub>10</sub> F-ratio for times			
< 10,000 years			
(year/m)			
Mean	5.035	5.103	
Median	4.989	5.039	
Variance	0.619	0.576	
5 <sup>th</sup> percentile	3.813	3.949	
25 <sup>th</sup> percentile	4.489	4.569	
75 <sup>th</sup> percentile	5.536	5.592	
95 <sup>th</sup> percentile	6.383	6.451	

Table 4-5. Summary statistics by repository level for the Aberg Base Case. Results for 100 realisations of 120 starting positions, a flow porosity of  $\epsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.

# 5 Variant Cases

Table 5-1 summarises the Base Case (the reference case for comparison) and the 5 variant cases evaluated for this study. Each variant corresponds to a possible interpretation of site hydrogeology, and is evaluated to address the acknowledged uncertainties. These are summarised as:

- Base Case (presented in Section 4.0, this represents the expected site conditions);
- Variant 1: Boundary condition variants;
- Variant 2: Upscaling of hydraulic conductivities;
- Variant 3: Anisotropic variogram of hydraulic conductivities;
- Variant 4: Conditional simulation of hydraulic conductivities; and
- Variant 5: Deterministic simulation.

The base case is discussed thoroughly in Section 4. The motivation and reasoning for each case is provided in the introduction of the sections corresponding to each case.

Case	Boundary conditions	Cell size		Hydraulic con	ductivity field		Conditioning on K	Remarks
	Obtained from	1	Scaling rule	Geostatistical model	Hydraulic units	EDZ/Backfill	on heads	
Base	TR 97-09, special case deliv_971129	25 m	Walker et al	Exponential isotropic Variance 2.7 Practical range 97 m	CD: SCD1 (Walker) RD: SRD1-5 (Walker)	No/10 <sup>-10</sup> m/s	No	BC for base case similar to SKB TR 97-09 (Appendix B)
Variant #1 Boundary Conditions 1.1; 1.2; 1.3; 1.4	TR 97-09 and some variants of the Base Case (5)	25 m						BC study for single realisation.
Variant #2 Upscaling		50 m		Variance=2.24				
Variant #3 Anisotropic variogram		25 m		Anisotropic variogram model (practical range ratio of) Variant 3.1=1:2:1 Variant 3.2=1:10:1	CD: Exclusion of NNW zones			Base Case BC
Variant #4 4.1 unconditional, 4.2 conditional		25 m		Variance = 3.14 Practical range = 122 m	No fracture zones included explicitly.			Pure stochastic continuum model. Geostatistical analysis using all data.
Variant #5 Deterministic		25 m	100 m Scale	Variance=0				Deterministic case

 Table 5-1. Summary of Base Case and Variant Cases analysed in Aberg site-scale modelling study.

# 5.1 Boundary Conditions

As was noted in Section 3.0, this study uses a nested modelling approach, with a regional model providing the site-scale boundary conditions. The regional model of Svensson (1997a) originally included the salinity dependence in the simulations, but that regional model cannot be used directly to provide boundary heads to HYDRASTAR, which is unable to simulate salinity. Svensson (1997a) also used a single realisation of the hydraulic conductivity field as the reference (base) case. Although this results in flow fields that have an intuitively attractive heterogeneity, the boundary heads would change if a different realisation of hydraulic conductivities were used. For the purposes of this model, therefore, the regional model of Svensson (1997a) was rerun for the Base Case using a deterministic hydraulic conductivity field and freshwater conditions (Appendix B). However, there are several possible methods for calculating and transferring boundaries between the regional and site-scale models, including:

- 1.1 Use a regional model with a deterministic, effective hydraulic conductivity and freshwater conditions (i.e., a single realisation of the Base Case, as discussed in Section 4.1).
- 1.2 Use a regional model with a single stochastic realisation of hydraulic conductivity and the observed salinity. Convert the resulting boundary pressures and salinities to environmental freshwater heads.
- 1.3 Use a regional model with a single stochastic realisation of hydraulic conductivity and freshwater conditions.
- 1.4 Avoid the regional model entirely and use the observed watertable/sea level and hydrostatic conditions directly in the site scale model as simplified boundary conditions.

The purpose of these variants is to determine the sensitivity of the site-scale model results to other approaches to transferring boundary conditions. Each variant uses the same hydraulic conductivity realisation for the site-scale model, resetting the boundary heads as necessary. The effect of these boundary conditions are evaluated by comparing the travel time, canister flux and F-ratio.

## 5.1.1 Deterministic Regional Model, Freshwater

This variant case begins with a single realisation of the Base Case to be used for comparison to all the boundary condition variants. That is, the first realisation uses boundary conditions derived from the Svensson (1997a) regional model rerun with a deterministic hydraulic conductivity field. The effective hydraulic conductivity,  $K_e$ , is assigned to the regional-scale RD and CD as suggested in Walker et al. (1997b). Unlike the Svensson (1997a) model, this regional model uses freshwater conditions to calculate the boundary heads. The resulting hydraulic heads are transferred to the site-scale model via linear interpolation (Appendix B).



Figure 5.1-1 shows the exit locations for all starting positions in the single realisation of the site-scale model.

Figure 5.1-1. Exit locations for Aberg Variant 1.1 (deterministic, freshwater regional model). Results for a single realisation of the Base Case and 120 starting positions. (Äspö local coordinate system, scale in metres).

## 5.1.2 Stochastic Regional Model, Salinity Dependent

This case uses the Base Case of the Svensson (1997a) regional model to calculate the boundary heads for the site-scale model. That regional model used a single realisation of a stochastic hydraulic conductivity field under salinity dependent conditions to calculate the boundary heads. The resulting hydraulic heads transferred to the site-scale model as depth-integrated environmental heads and linear interpolation (Appendix B).

Figure 5.1-2 shows the exit locations for all starting positions in the single realisation of the site-scale model.



Figure 5.1-2. Exit locations for Aberg Variant 1.2 (stochastic, salinity dependent regional model). Results for a single realisation of the Base Case and 120 starting positions. (Äspö local coordinate system, scale in metres).

## 5.1.3 Stochastic Regional Model, Freshwater

This case uses the Svensson (1997a) regional model under freshwater conditions to calculate the boundary heads for the site-scale model. That regional model was a single realisation of a stochastic hydraulic conductivity field, similar to that the boundary conditions used by Widén and Walker (1998). The resulting hydraulic heads transferred to the site-scale model via linear interpolation (Appendix B).

Figure 5.1-3 shows the exit locations for all starting positions in the single realisation of the site-scale model.



*Figure 5.1-3. Exit locations for Aberg Variant 1.3 (stochastic, freshwater regional model). Results for a single realisation of the Base Case and 120 starting positions. (Äspö local coordinate system, scale in metres).* 

## 5.1.4 Simplified Boundaries

This variant examines the possibility of avoiding the nested modelling approach, and attempts to set boundary conditions using only the observed topography and simplified boundaries at depth. The upper constant head boundary is taken from the Äspö site digital terrain model and the empirical relationship of surface elevation to groundwater table elevation. Two variants are tested for the lateral and bottom boundary conditions, the first being to use no flow boundary conditions on the vertical and bottom sides, called variant 1.4b. Figure 5.1-4 presents the resulting exit locations for these boundary conditions for realisation number 1. In this case, the exit locations are widely dispersed over the model surface, and 5 of the stream tubes (4%) failed to exit the upper surface of the model.



Figure 5.1-4. Exit locations for Aberg Variant 1.4b (simplified boundary conditions with no flow conditions on the vertical sides and bottom). Results for a single realisation of the Base Case and 120 starting positions. (Äspö local coordinate system, scale in metres).

Variant 1.4c attempts to set boundary conditions using the observed topography on the model's upper surface, hydrostatic head on the lateral surfaces, and no flow on the bottom surface. Figure 5.1-5 presents the resulting exit locations for these boundary conditions for realisation number 1. The exit locations are widely dispersed over the model surface, and 30 stream tubes (25%) failed to exit the upper surface of the model.



Figure 5.1-5. Exit locations for Aberg Variant 1.4c (simplified boundary conditions with hydrostatic head on the vertical sides and no flow conditions on bottom). Results for a single realisation of the Base Case and 120 starting positions. (Äspö local coordinate system, scale in metres).

#### 5.1.5 Comparison

Figures 5.1-6 and 5.1-7 present the hydraulic head distributions on the southern surface of the model. The head distributions for variants 1.1, 1.2 and 1.3 are relatively similar, where variant 1.4c is strikingly different. These differences and similarities are reflected in the performance measure statistics for the 120 start positions for each method of assigning boundary conditions (Table 5.1-1). Comparing the results, note that all three variants for transferring heads from the regional model give rather similar results (i.e. variants 1.1, 1.2 and 1.3 have similar travel time, canister flux and F-ratios). Variant 1.4 (simplified boundary conditions based on topography) gives rather different results in comparison to the first variants. Likewise, Table 5.1-2 indicates that these similarities and differences are seen in the boundary fluxes as well. The comparative plots of  $log_{10}$ travel time and  $log_{10}$  canister flux histograms (Figures 5.1-8 and 5.1-9) show that both the travel times and canister fluxes are quite different for the simplified boundary conditions (variants 1.4b and 1.4c). This suggests that the regional flow pattern imparted by the nested modelling does have important effects.



Figure 5.1-6. Head boundary conditions for Aberg Variant 1, on the southern model surface for a) Variant 1.1, b) Variant 1.2, and c) Variant1.3 (freshwater hydraulic head in metres).

This variant does have its limitations, however, since only constant head (Dirichlet) boundaries are investigated. A useful extension of this variant would be to investigate the effects of changing to constant flux (Neuman) or third-type boundaries. Unlike constant head boundaries, constant flux and third-type boundaries do not restrict the head variability on the boundaries and therefore would allow greater head variance in the domain. Such alternative boundary conditions are beyond the current capabilities of HYDRASTAR, however.



*Figure 5.1-7. Head boundary conditions for Aberg Variant 1.4c, on the southern model surface. (Variant 1.4b used no flow condition on all vertical sides). (Freshwater hydraulic head in metres).* 

	$1 \times 10^{-4}$ and flow-wetted surface $a_r = 1.0 \text{ m}^2/\text{m}^3$ .							
	Median log <sub>10</sub> t <sub>w</sub> for times < 10,000 years (variance)	Median log <sub>10</sub> q <sub>c</sub> for all times (variance)	Median log <sub>10</sub> F-ratio for times < 10,000 years (variance)	Percent of stream tubes failing to exit				
Base Case	1.015	-2.736	5.015	0.5				
	(0.599)	(0.935)	(0.599)					
Variant 1.1	0.875	-2.667	4.875	0				
	(0.578)	(0.735)	(0.578)					
Variant 1.2	0.947	-2.667	4.947	0.9				
	(0.513)	(0.733)	(0.513)					
Variant 1.3	0.912	-2.659	4.912	0				
	(0.523)	(0.747)	(0.523)					
Variant 1.4b	1.951	-3.374	5.951	4.2				
	(0.517)	(0.872)	(0.517)					
Variant 1.4c	1.485	-3.316	5.485	25				
	(0.580)	(0.8059	(0.580)					

Table 5.1-1. Comparison of median performance measures within Aberg Variant 1. Results for a single realisation of 120 starting positions, a flow porosity of  $\epsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ .

		Net flux through subdomain (m <sup>-3</sup> /s x 10 <sup>-3</sup> )				
Model	Case 1.1	Case 1.2	Case 1.3	Case 1.4b	Case 1.4c	
Surface						
West	6.81 (in)	6.81 (in)	6.15 (in)	0	1.90 (in)	
East	1.16 (in)	0.0703 (out)	0.453 (in)	0	0.152 (in)	
South	0.349 (in)	0.190 (in)	0.564 (in)	0	0.738 (in)	
North	0.363 (in)	0.474 (in)	0.372 (in)	0	0.141 (out)	
Bottom	0.826 (in)	0.243 (in)	0.744 (in)	0	0	
Тор	9.50 (out)	7.65 (out)	8.32 (out)	$1.45^{-10^{-5}}$ (in)	2.650 (out)	
Total inflow	9.508	7.7217	8.283	$1.45^{\cdot}10^{-5}$	2.7890	
Total	9.500	7.7154	8.320	0	2.7907	
outflow						
Mass	0.008	0.0063	-0.037	$1.45^{\cdot}10^{-5}$	-0.0017	
balance (In-						
Out)						

 Table 5.1-2.
 Boundary flux comparison within Aberg Variant 1.



Figure 5.1-8. Floating histograms of  $log_{10}$  travel time for Aberg Variant 1, normalised to the number of stream tubes less than 10,000 years. Results for a single realisation of 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



*Figure 5.1-9. Floating histograms of log*<sub>10</sub> *canister flux for Aberg Variant 1.* 

# 5.2 Upscaling

Hydraulic conductivity is thought to be scale dependent, but current research debates the correct method for scaling field measurements for use in continuum modelling. The Base Case uses the observed Äspö scale dependence to determine the geometric mean of hydraulic conductivity for the finite difference blocks, and the Moye's formula regularisation to determine the variogram. The resulting parameters are used to simulate hydraulic conductivity fields at the 25 m grid scale (Walker et al., 1997b). It is important to evaluate the uncertainty of this upscaling method on the model results.

This variant examines the affect of changing the model calculation scale to a 50 m regular grid with commensurate rescaling of the parameters for simulating the hydraulic conductivity field. Appendix C.2.2 summarises the geostatistical inference of a 50 m scale model for hydraulic conductivity. The SKB code INFERENS was used to infer a regularised variogram model for the 50 m scale, based on the 3 m packer tests in the rock mass domain. Results of this analysis indicated the following variogram model for the 50 m grid scale (Figure 5.2-1):

- Exponential model, isotropic,
- Practical range of 111 m, and
- Zero nugget,  $\log_{10}$  K variance 2.24.

The SRD and SCD are treated as step changes in the geometric mean of block conductivities (0 order trends in  $K_b$ ), with values provided in Table 5.2-1.



*Figure 5.2-1. Semivariogram of Aberg log*<sub>10</sub> *hydraulic conductivity for rock domain.* 3 m data in rock domain, regularised to 50 m and fitted via INFERENS.

hydra	hydraulic conductivities change by a factor of 1/10.							
Parameter	Measured	Base Case 25 m Scale	Variant 2 50 m Scale	Variant 5 Deterministic				
Variogram								
model								
Total variance	2.84	2.72	2.24	0				
Practical range	112	97	111	-				
Mean Log <sub>10</sub> K								
SRD 1	-8.7	-8.0	-7.8	-7.6				
SRD 2	-7.8	-7.1	-6.9	-6.6				
SRD 3	-9.5	-8.8	-8.5	-8.3				
SRD 4	-7.6*	-7.5	-7.3	-7.1				
SRD 5	-8.3	-7.6	-7.4	-7.1				
other	-9.3	-8.5	-8.3	-8.1				
EW-1N	-7.3	-7.8	-7.5	-7.3				
EW-1S	-6.1	-6.6	-6.4	-6.1				
EW-3	-5.8	-6.3	-6.0	-5.8				
EW-7	-5.2	-5.7	-5.4	-5.2				
NE-1	-5.0	-5.5	-5.2	-5.0				
NE-2	-7.1	-7.6	-7.3	-7.1				
NE-3	-5.2	-5.7	-5.5	-5.2				
NE-4	-6.1	-6.6	-6.4	-6.1				
NNW-1	-6.3	-6.7	-6.5	-6.3				
NNW-2	-5.6	-6.0	-5.8	-5.6				
NNW-4	-4.8	-5.3	-5.1	-4.8				
NNW-5	-7.0	-7.5	-7.2	-7.0				
NNW-7	-6.6	-7.1	-6.9	-6.6				
NNW-8	-6.3	-6.8	-6.5	-6.3				
<b>NW-1</b>	-7.8	-8.3	-8.0	-7.8				

Table 5.2-1. Upscaled Parameters for Base Case, Variant 2 and Variant 5. Measured parameters shown for comparison. Below z = -600 masl, the hydraulic conductivities change by a factor of 1/10.

\* Inferred from calibration at 20 m scale, Svensson (1997a).

Tables 5.2-2 and 5.2-3 summarise the consequences of changing the grid resolution and rescaling the conductivities. In comparison to the Base Case, the median travel time is reduced from 10 to 5.8 years and the median canister flux is increased from  $1.9 \times 10^{-3}$  to  $4.0 \times 10^{-3}$  m/yr. The variances of both of these performance measures are reduced by approximately 30% (Table 5.2-4). The distributions of both travel time and canister flux for this variant are significantly different from the comparable distributions of the Base Case (Appendix A.2). The boundary fluxes are slightly increased with respect to the Base Case, but five realisations may be insufficient for the mean fluxes to have stabilised.

	All V		Travel Times>10,000 years deleted			
	Log <sub>10</sub> t <sub>w</sub>	Log <sub>10</sub> q <sub>c</sub>	Log <sub>10</sub> F-	Log <sub>10</sub> t <sub>w</sub>	Log <sub>10</sub> q <sub>c</sub>	Log <sub>10</sub> F-ratio
			ratio			
Mean	0.825	-2.449	4.825	0.814	-2.448	4.814
Median	0.770	-2.400	4.770	0.766	-2.398	4.766
Variance	0.456	0.560	0.456	0.426	0.559	0.426
5th percentile	-0.187	-3.767	3.813	-0.187	-3.766	3.813
25th	0.354	-2.933	4.354	0.352	-2.931	4.352
percentile						
75th	1.247	-1.912	5.247	1.242	-1.912	5.242
percentile						
95th	1.964	-1.311	5.964	1.940	-1.310	5.940
percentile						

Table 5.2-2. Summary statistics for Aberg Variant 2. Results for 100 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.

# Table 5.2-3. Boundary flux consistency for Aberg Base Case, Variant 2 and<br/>regional models.

Model Surface	Regional	Base Case	Variant 2
	-	25 m Scale	50 m Scale
West	13.7 (in)	4.92 (in)	6.66 (in)
East	0.916 (in)	0.77 (in)	0.730 (in)
South	1.81 (in)	0.846 (in)	0.489 (out)
North	0.625 (in)	0.538 (in)	0.340 (in)
Bottom	0.374 (in)	1.03 (in)	1.11 (in)
Тор	18.1 (out)	8.11 (out)	8.34 (out)
Total Inflow	17.425	8.1137	8.834
Total Outflow	18.1	8.11	8.825
Mass balance (In – Out)	-0.675	-0.0037	0.009

	Median log <sub>10</sub> t <sub>w</sub> for times < 10,000 years (variance)	Median log <sub>10</sub> q <sub>c</sub> for all times (variance)	Median log <sub>10</sub> F- ratio for times < 10,000 years (variance)
Base Case	1.015	-2.736	5.015
	(0.599)	(0.935)	(0.599)
Variant 2	0.766	-2.400	4.766
	(0.426)	(0.560)	(0.426)

Table 5.2-4. Comparison of median performance measures of Aberg Variant 2 and Base Case. Results for 100 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ .

While the relative agreement of the boundary fluxes from the 25 to 50 m scales suggests that the upscaling method is adequate, the disagreement of the median travel times and canister fluxes suggests that the method is not effective. Indelman and Dagan (1993) suggested that upscaling should be tied to the grid shape, size and density with respect the integral scale of correlation. McKenna and Rautman (1996) studied various upscaling algorithms and confirmed that the behaviour of upscaling approaches could be quite complex, depending on the grid density relative to the integral scale of correlation. Given differences between the site-scale boundary fluxes, it is unsurprising that the median travel times also differ for the 25 and 50 m scales. The increase in boundary flux and decrease in travel time suggest that the upscaling algorithm may excessively increase the effective conductivity of the domain.

The reduced variance of both the travel times and canister fluxes is appropriate, given the reduced input variance for the  $log_{10}$  hydraulic conductivities. Figure 5.2-2 presents the exit locations for this variant, whose general pattern is very similar to that of the Base Case. The locations appear to be slightly more dispersed than in the Base Case, which is attributed to the coarser grid of this variant.



Figure 5.2-2. Exit locations for Aberg Variant 2 (upscaling to 50 m). Results for 100 realisations of 120 starting positions. (Äspö local coordinate system, scale in metres).

# 5.3 Anisotropic Variogram

Site investigations at Äspö and at various other locations in Sweden suggest that the host rocks may exhibit hydraulic anisotropy, with a preferred direction aligned with the principal axes of rock stress (Ericsson and Ronge, 1986; Rhén et al., 1997). Although the current version of HYDRASTAR (1.7.2) does not allow for block-scale anisotropy, the hydraulic anisotropic of a stochastic continuum model is related to the scale dependence of hydraulic conductivity. For example, Gutjahr, et al. (1978) found that a large-scale anisotropic hydraulic conductivity evolves from isotropic (scalar) point values of hydraulic conductivities with an anisotropic spatial variogram. That is, the anisotropic variogram of isotropic point hydraulic conductivities creates a large-scale anisotropy is also tied to the complex problem of upscaling and the determination of block conductivities (Renard and de Marsily, 1997).

This variant uses stochastic anisotropy to examine the effects of hydraulic anisotropy on the model predictions. Bergman and Walker (1998) briefly examined this approach via numerical experiments using HYDRASTAR. They found that the analytical solutions of Gelhar and Axness (1983) could estimate the stochastic anisotropy ratio needed to produce a desired anisotropic effective hydraulic conductivity for low variances (less than  $\sigma^2_{\log K} = 0.19$ ). For higher variances, Bergman and Walker (1998) found that the analytical solutions might not be useful in estimating the necessary stochastic anisotropy ratio. They found that increasing the variance would allow using a relatively low stochastic anisotropy ratio to produce much larger effective anisotropy ratios. Bergman and Walker (1998) also suggested that typical HYDRASTAR model grids used in SR 97 might not be sufficiently dense with respect to the integral scale to produce the desired anisotropic effective conductivity.

Applying the analytical solutions of Gelhar and Axness (1983) to field data, Neuman and Depner (1988) determined a stochastically anisotropic variogram model for a given anisotropic effective hydraulic conductivity. Appendix C.1 summarises the application of the Neuman and Depner (1988) approach to the Äspö data and the large-scale anisotropy suggested for Äspö by Rhén, et al. (1997). The Neuman and Depner approach indicated the anisotropy ratio of 1.5:2:1 in the Vertical:NW:NE directions. However, the relative coarseness of the model grid would not be able to adequately produce the indicated shortened range in the NE, forcing this study to simplify this ratio to 1:2:1. If the vertical range is preserved, the practical ranges of correlation are Vertical:NW:NE = 97 m:194 m:97 m. This simplified stochastic anisotropy should be expected to produce fields with a one-dimensional anisotropy, with a major axis toward the NW. Variant 3.1 evaluates this 1:2:1 ratio with 50 realisations, and Variant 3.2 examines the uncertainty of this approach by repeating the simulations with a ratio of 1:10:1.

Figure 5.3-1 presents the conductivity field at the upper repository level for Variant 3.1, which uses a variogram anisotropy of 1:2:1. The overall effect is to create rough ellipsoids of conductivity, with the long axes parallel to the major axis of anisotropy

(northwest-southeast; see Figure 5.3-1a). A vertical cross-section through the field (Figure 5.3-1b) reveals that there is no comparable continuity in the vertical direction, as might be expected with subvertical fracturing. This confirms that the simplified anisotropy ratio creates a one-dimensional anisotropy, whose effects are discussed further below.



Figure 5.3-1. Log<sub>10</sub> hydraulic conductivity for one realisation of Aberg Variant 3.1 (anisotropic variogram), on a) upper model surface and b) on southern model surface. (Äspö local coordinate system, scale in metres).

Although the exit locations (Figure 5.3-2) are similar to those of the Base Case, Figure 5.3-3 shows that the flow pattern is changed, with stream tubes reorganised parallel to the major axis of anisotropy. Table 5.3-1 indicates that, in comparison to the Base Case, the median travel time is only slightly increased from 10 to 12 years and the median canister flux is only slightly decreased from  $1.9 \times 10^{-3}$  to  $1.6 \times 10^{-3}$  m/yr. The shapes of both the travel time and canister flux distributions for this variant are significantly different from those of the Base Case (Appendix A.2). Although the change in flow pattern is consistent with the findings of Svensson (1997a), the similarity of median travel times between this variant and the Base Case is not consistent with Svensson (1997a). Possible causes for this inconsistency are discussed below.

Table 5.3-1. Summary statistics for Aberg Variant 3.1. Results for 50 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in **bold** are discussed in text.

All values				Travel Times > 10,000 years			
				deleted			
	Log <sub>10</sub>	Log <sub>10</sub>	Log <sub>10</sub> F-	Log <sub>10</sub> t <sub>w</sub>	Log <sub>10</sub> q <sub>c</sub>	Log <sub>10</sub> F-	
	tw	q <sub>c</sub>	ratio	_		ratio	
Mean	1.156	-2.859	5.156	1.140	-2.855	5.140	
Median	1.099	-2.803	5.099	1.091	-2.801	5.091	
Variance	0.720	1.034	0.720	0.677	1.023	0.677	
5 <sup>th</sup> percentile	-0.161	-4.635	3.839	-0.161	-4.623	3.839	
25 <sup>th</sup> percentile	0.568	-3.524	4.568	0.565	-3.518	4.565	
75 <sup>th</sup> percentile	1.694	-2.129	5.694	1.681	-2.129	5.681	
95 <sup>th</sup> percentile	2.638	-1.309	6.638	2.581	-1.310	6.581	



Figure 5.3-2. Exit locations for Aberg Variant 3.1 (anisotropic variogram). Results for 50 realisations of 120 starting positions. (Äspö local coordinate system, scale in metres).



a) Plan view



b) Elevation view, from South



c) Elevation view, from East

Figure 5.3-3. Stream tubes for realisation number 1 of Aberg Variant 3.1 (anisotropic variogram). The y-positive axis of a) points in the direction of Äspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

Figure 5.3-4 presents the  $\log_{10}$  hydraulic conductivity field for Variant 3.2, with a variogram anisotropy of 1:10:1. Relative to the  $\log_{10}$  hydraulic conductivity field of Variant 3.1, the ellipsoidal features are more prominent and much longer, but likewise show little vertical continuity. Figure 5.3-5 shows that the exit locations are shifted to the southeast, and the stream tubes of Figure 5.3-6 are now strongly oriented along the northwest-southeast axis.

Table 5.3-2 indicates that, in comparison to the Base Case, the median travel time is slightly increased from 10 to 11 years and the median canister flux is slightly decreased from  $1.9 \times 10^{-3}$  to  $1.8 \times 10^{-3}$  m/yr. The variances of both of these performance measures are reduced by 30% relative to the Base Case, and the shape of the distributions for this variant is significantly different from those of the Base Case (Appendix A.2).

Table 5.3-3 summarises the results of the two anisotropy ratios considered in this variant and compares them to the Base Case. The median travel times and median canister fluxes are nearly the same for both anisotropy ratios and also very similar to the median travel time and median canister flux of the Base Case. As noted above, the similarity of these isotropic and anisotropic cases is not consistent with the findings of Svensson (1997a), which suggested that travel times would be strongly affected by anisotropy. This inconsistency can be partly attributed to the use of a simplified stochastic anisotropy ratio in these variants, which creates fields with a single direction of continuity (northwest-southeast). As discussed above and in Appendix C.3, this simplification is forced by the coarseness of the model grid, resulting in fields that have an effective conductivity that is anisotropic in one-dimension with the major axis perpendicular to the upward gradient. Such an approach is very different from the 3-dimensional block-scale hydraulic anisotropy used by Svensson (1997a), whose increased vertical conductivity is aligned with the upward gradient.

For both anisotropy ratios considered in this variant the only apparent difference relative to the Base Case is an increase in the variance of the performance measures and a reorganisation of the stream tubes. This is attributed to the interception of stream tubes by the large scale structures represented by the ellipsoids of hydraulic conductivity.



Figure 5.3-4. Log<sub>10</sub> hydraulic conductivity for one realisation of Aberg Variant 3.2 (anisotropic variogram), on a) upper model surface and b) on southern model surface. (Äspö local coordinate system, scale in metres).

Sulla	.v m /m .	i voiu ai e (	iiscusseu iii	іслі.			
	All values			Travel Times > 10,000 years			
					deleted		
	$Log_{10}$	$\mathbf{Log}_{10}$	$\mathbf{Log}_{10} \mathbf{F}$ -	$\mathbf{Log}_{10} \mathbf{t}_{\mathbf{w}}$	$\mathbf{Log}_{10} \ \mathbf{q_c}$	$Log_{10}F$ -	
	$\mathbf{t}_{\mathbf{w}}$	q <sub>c</sub>	ratio			ratio	
Mean	1.111	-2.770	5.111	1.086	-2.768	5.086	
Median	1.043	-2.733	5.043	1.032	-2.737	5.032	
Variance	0.794	1.171	0.794	0.728	1.153	0.728	
5 <sup>th</sup> percentile	-0.229	-4.604	3.771	-0.234	-4.588	3.766	
25 <sup>th</sup> percentile	0.496	-3.484	4.496	0.490	-3.483	4.490	
75 <sup>th</sup> percentile	1.656	-2.016	5.656	1.635	-2.020	5.635	
95 <sup>th</sup> percentile	2.667	-1.072	6.667	2.582	-1.070	6.582	

Table 5.3-2. Summary statistics for Aberg Variant 3.2. Results for 50 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.



Figure 5.3-5. Exit locations for Aberg Variant 3.2 (anisotropic variogram). Results for 50 realisations of 120 starting positions. (Äspö local coordinate system, scale in metres).



a) Plan view



b) Elevation view, from South



c) Elevation view, from East

Figure 5.3-6. Stream tubes for realisation number 1 of Aberg Variant 3.2 (anisotropic variogram). The y-positive axis of a) points in the direction of Äspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

t	time statistics computed for $t_w$ less than 10,000 years.							
	Median log <sub>10</sub> t <sub>w</sub> (variance)	Median log <sub>10</sub> q <sub>0</sub> (variance)	9 Median log <sub>10</sub> F- ratio (variance)	Percent of stream tubes failing to exit				
Base Case	1.015	-2.736	5.015	0.4833				
	(0.599)	(0.935)	(0.599)					
Variant 3.1	1.091	-2.803	5.091	0.5833				
	(0.677)	(1.034)	(0.677)					
Variant 3.2	1.032	-2.733	5.032	0.8667				
	(0.728)	(1.171)	(0.728)					

Table 5.3-3. Comparison of median performance measures Aberg Base Case and Variant 3. Results for 50 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Travel time statistics computed for  $t_w$  less than 10,000 years.

# 5.4 Conditional Simulation

The Base Case of this study (Section 4) uses unconditional geostatistical simulation to create the hydraulic conductivity fields, and includes fracture zones as deterministic zones of increased mean log<sub>10</sub> hydraulic conductivity. This is not the only HYDRASTAR option for creating the hydraulic conductivity fields. For example, HYDRASTAR can also condition the fields on observed hydraulic conductivity measurements via conditional simulation, with ordinary kriging to imply fracture zones via kriging neighbourhoods. Conditional simulation was not used in the Base Case, however, because the relatively short correlation length implies that the main effect of conditioning is to control the mean of the kriging neighbourhood. HYDRASTAR also can condition the hydraulic conductivity fields by calibrating the fields to observed head values. This was not used for the Base Case because calibration demands an extreme level of computational effort.

Although conditioning on K measurements was not used for the Base Case, it is important to evaluate the effects of conditioning on model results. Two variants are considered:

- Variant 4.1: Unconditional simulation and
- Variant 4.2: Conditional simulation

Note that the above variants are without deterministic fracture zones. This is a consequence of a conflict between the defined zones, the conditioning data and kriging neighbourhoods. In principle, it is possible to define kriging neighbourhoods that corresponding to zones such that conditioning hydraulic conductivity measurements are assigned to the appropriate RD and CD domains. In practice, however, it is not possible to use such detailed kriging neighbourhoods in HYDRASTAR 1.7.2, and therefore this study does not examine the joint effect of deterministic zones and conditioning on hydraulic conductivity measurements.

These variants use a simplified geostatistical model, with a variogram fitted to all of the hydraulic conductivities of the 3 m packer test data within the site-scale model domain. The variants use no deterministic zones at all and use a single kriging neighbourhood to allow conditioning the simulated hydraulic conductivity fields to measured hydraulic conductivities. In addition, this variant uses the Moye's-based upscaling algorithm to determine the expectation and variogram of the upscaled hydraulic conductivities. (See Appendix C). This approach yields the following geostatistical model:

- A mean  $\log_{10}$  hydraulic conductivity = -7.7 m/s,
- Isotropic exponential variogram model, total variance = 3.11, and
- Practical range of 122 m.

Both the variance and the  $log_{10}$  hydraulic conductivity are increased relative to the Base Case rock mass (SRD) parameters. These increases can be attributed to the inclusion of the CD data in the data used in the INFERENS variogram analysis.

#### 5.4.1 Unconditional Simulation

This variant is simulated without fracture zones and without conditioning data. Its primary purpose is to establish the changes in the results that arise from removing the fracture zones. It is therefore useful in comparison to the Base Case and for the conditional simulation variants.

The  $\log_{10}$  hydraulic conductivity field appears to be unstructured, as expected with the removal of the deterministic fracture zones (Figure 5.4-1). The exit locations are nearly random, controlled only by the recharge under the land surface (Figure 5.4-2). Likewise, the stream tubes travel randomly in the domain, and show no organisation along conductive features (Figure 5.4-3).



*Figure 5.4-1.* Log<sub>10</sub> hydraulic conductivity at repository level for Aberg Variant 4.1 (unconditional simulation). (Äspö local coordinate system, scale in metres).



Figure 5.4-2. Exit locations for Aberg Variant 4.1 (unconditional simulation). Results for 50 realisations of 120 starting positions. (Äspö local coordinate system, scale in metres).



a) Plan view



b) Elevation view, from South



c) Elevation view, from East

Figure 5.4-3. Stream tubes for realisation number 1 of Aberg Variant 4.1 (unconditional simulation). The y-positive axis of a) points in the direction of Äspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .

The performance measure statistics for this variant are given in Table 5.4-1. Comparing this variant versus Base Case (Section 4.3), the median travel time is shortened from 10 to 4.1 years, and its variance is reduced from 0.599 to 0.465. The median canister flux is increased from  $1.9 \times 10^{-3}$  to  $6.7 \times 10^{-3}$  m/yr. Both the travel time and canister flux distributions for this variant are significantly different from those of the Base Case (Appendix A.2). As anticipated, the travel paths show no organisation around linear patterns associated with fracture zones. One might anticipate that removing the deterministic zones might delete the fast paths. However, recall that K<sub>g</sub> and the variance of  $\log_{10} K$  have increased relative to the Base Case. As is discussed briefly in Section 5.3, the increases of both the mean and variance of  $\log_{10} K$  tend to increase the effective conductivity of the domain (Gutjahr et al., 1978), resulting in reduced travel times. Also note that the travel time variance is reduced even though the input variance of  $\log_{10} K$  has been increased (from 2.7 to 3.1). This travel time variance increase is attributed to removing the fracture zones (SCD), such that only a single domain is encountered by any given stream tube.

surf	$.0 \text{ m}^2/\text{m}^3.$	n bold are o	discussed in	text.			
	All values			Travel Times > 10,000 years			
				deleted			
	$\mathbf{Log}_{10}$	$\mathbf{Log}_{10}$	$Log_{10}$ F-	$\mathbf{Log}_{10} \mathbf{t}_{\mathbf{w}}$	$\mathbf{Log}_{10}  \mathbf{q_c}$	$\mathbf{Log}_{10} \mathbf{F}$ -	
	tw	qc	ratio			ratio	
Mean	0.673	-2.232	4.673	0.661	-2.233	4.661	
Median	0.620	-2.173	4.620	0.617	-2.174	4.617	
Variance	0.502	0.891	0.502	0.465	0.890	0.465	
5 <sup>th</sup> percentile	-0.387	-3.898	3.613	-0.387	-3.898	3.613	
25 <sup>th</sup> percentile	0.196	-2.847	4.196	0.196	-2.848	4.196	
75 <sup>th</sup> percentile	1.089	-1.564	5.089	1.080	-1.566	5.080	
95 <sup>th</sup> percentile	1.880	-0.810	5.880	1.842	-0.810	5.842	

Table 5.4-1 Summary statistics for Aberg Variant 4.1. Results for 50 realisations of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.

## 5.4.2 Conditional Simulation

As with Variant 4.1, this variant is simulated without fracture zones and a mean  $log_{10}$  hydraulic conductivity of -7.7, a variance of 3.11 and a practical range 122 m. In this variant, however, the 3 m-interpreted hydraulic conductivities are included as conditioning data in the simulated conductivity fields. The purpose of this variant is to establish the changes in the results that arise from including conditioning data. It should be compared to Variant 4.1, the unconditional simulation. Unlike the Base Case, which relies on interference test data for the conductivity of the deterministic fracture zones, this simulation uses only the 3 m packer test data.

The  $log_{10}$  hydraulic conductivity field appears to be identical to the unconditional case. Figure 5.4-4 presents the  $log_{10}$  hydraulic conductivities at the upper repository level, which shows that no large-scale structures have been created as a result of including measurements in the fracture zones. This is attributed to the relatively short practical range of correlation of 122 m and the wide data spacing. Similar to the unconditional case in this variant, the exit locations are nearly random, controlled only by the recharge under the land surface (Figure 5.4-5). Likewise, the stream tubes travel randomly in the domain, and show no organisation along conductive features (Figure 5.4-6).

The performance measure statistics for this variant are given in Table 5.4-2. Comparing this variant versus the unconditional simulation (Section 5.4.1), the median travel times are slightly decreased to 3.2 years, and the variance is slightly increased to 0.512. The median canister flux is slightly increased to 8.2 x  $10^{-3}$  m/year (Table 5.4-3). Both the travel time and canister flux distributions for this variant are significantly different from those of the Base Case (Appendix A.2). It is possible that these changes reflect the implicit inclusion of conductive structures. The stream tubes have a similar degree of disorganisation as those of Variant 4.1.

# Table 5.4-2. Summary statistics for Aberg Variant 4.2. Results for 50 realisations of 120 starting positions, a flow porosity of $\varepsilon_f = 1 \times 10^{-4}$ and flow-wetted surface $a_r = 1.0 \text{ m}^2/\text{m}^3$ . Statistics in bold are discussed in text.

	All values			Travel Times > 10,000 years		
				deleted		
	$\mathbf{Log}_{10}$	$\mathbf{Log}_{10}$	$\mathbf{Log}_{10} \mathbf{F}$ -	$\mathbf{Log}_{10} \mathbf{t}_{\mathbf{w}}$	$\mathbf{Log}_{10} \ \mathbf{q_c}$	$\mathbf{Log}_{10} \mathbf{F}$ -
	tw	q <sub>c</sub>	ratio			ratio
Mean	0.575	-2.136	4.575	0.551	-2.137	4.551
Median	0.508	-2.087	4.508	0.502	-2.088	4.502
Variance	0.590	0.973	0.590	0.512	0.969	0.512
5 <sup>th</sup> percentile	-0.553	-3.827	3.447	-0.553	-3.825	3.447
25 <sup>th</sup> percentile	0.064	-2.780	4.064	0.061	-2.780	4.061
75 <sup>th</sup> percentile	1.027	-1.441	5.027	1.012	-1.444	5.012
95 <sup>th</sup> percentile	1.834	-0.627	5.834	1.786	-0.627	5.786

Table 5.4-3. Comparison of Base Case and Variant 4. Results for a single realisation of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ .

	Median log <sub>10</sub> t <sub>w</sub> for times < 10,000 years (variance)	Median log <sub>10</sub> c for all times (variance)	le Median log <sub>10</sub> F-ratio for times < 10,000 years (variance)
Base Case	1.015	-2.736	5.015
	(0.599)	(0.935)	(0.599)
Variant 4.1	0.617	-2.173	4.617
Unconditional	(0.465)	(0.891)	(0.465)
Variant 4.2	0.502	-2.087	4.502
Conditional	(0.512)	(0.973)	(0.512)



Figure 5.4-4. Log<sub>10</sub> hydraulic conductivity for one realisation at repository level for Aberg Variant 4.2 (conditional simulation). (Äspö local coordinate system, scale in metres).

( log m/s )



Figure 5.4-5. Exit locations for Aberg Variant 4.2 (conditional simulation). Results for 50 realisations of 120 starting positions. (Äspö local coordinate system, scale in metres).


a) Plan view



b) Elevation view, from South



c) Elevation view, from East

Figure 5.4-6. Stream tubes for realisation number 1 of Aberg Variant 4.2 (conditional simulation). The y-positive axis of a) points in the direction of Äspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

### 5.5 Deterministic Simulation

This variant is a simplified simulation of the site using a deterministic representation of the hydraulic conductivity field (i.e., the field has no random component and thus needs only one 'realisation'). The objectives of this simulation are to further evaluate the empirical upscaling and nested modelling, and to examine the effects of the large-scale heterogeneity (e.g., the fracture zones and rock blocks). As was discussed in Sections 4.2, 5.1 and Appendix C.2, choosing the appropriate hydraulic conductivities is complicated by the apparent scale dependence of hydraulic conductivity. We might choose to use exactly the same hydraulic conductivities as the regional model of Svensson (1997a; see also Appendix B), but the site scale model includes rock blocks and fracture zones that have no corresponding regional structures. As a compromise, this study uses the empirical upscaling rule (Appendix C.2) to determine the effective conductivity, Ke, for each rock unit. If the nested modelling and upscaling are consistent, the boundary fluxes should be approximately the same for the regional model, the Base Case and this deterministic variant. The parameters for this case were previously presented in Table 5.2-1, and represent as the effective conductivities of each unit. Note that for this variant, there is no block-scale variability (zero variance).

Table 5.5-1 summarises the results of this deterministic simulation in terms of the travel time, canister flux and F-ratio, averaged over all the starting positions. In comparison to the Base Case, the median travel time is increased from 10 to 12 years, and the median canister flux is increased from  $1.9 \times 10^{-3}$  to  $2.1 \times 10^{-3}$  m/yr (Table 5.5-2). The variances of both of these measures are dramatically reduced, as expected for a deterministic field.

	All values				
	$\mathbf{Log}_{10} \mathbf{t}_{\mathbf{w}}$	$\mathbf{Log}_{10} \ \mathbf{q_c}$	Log <sub>10</sub> F-ratio		
Mean	1.049	-2.708	5.049		
Median	1.074	-2.672	5.074		
Variance	0.273	0.192	0.273		
5 <sup>th</sup> percentile	0.260	-3.417	4.260		
25 <sup>th</sup> percentile	0.584	-3.028	4.584		
75 <sup>th</sup> percentile	1.386	-2.354	5.386		
95 <sup>th</sup> percentile	2.048	-2.094	6.048		

Table 5.5-1. Summary statistics for Aberg Variant 5. Results for 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and upper flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ . No stream tubes fail to exit the model surface in this variant. Statistics in bold are discussed in text.

Table 5.5-2. Comparison of median performance measures within Aberg Base Case, Variant 2 and Variant 5. Results for a single realisation of 120 starting positions, a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$  and flow-wetted surface  $a_r = 1.0 \text{ m}^2/\text{m}^3$ .

	Median log <sub>10</sub> t <sub>w</sub> for t	imes Median log <sub>10</sub> q <sub>c</sub> for	Median log <sub>10</sub> F-ratio for
	< 10,000 years (variance)	all times (variance)	times < 10,000 years (variance)
Base Case	1.015	-2.736	5.015
	(0.599)	(0.935)	(0.599)
Variant 2	0.766	-2.400	4.766
	(0.426)	(0.560)	(0.426)
Variant 5	1.074	-2.672	5.074
	(0.273)	(0.192)	(0.273)

Table 5.5-3 summarises the boundary fluxes; note that this deterministic variant under predicts the Base Case boundary fluxes by approximately a factor of ½ to 1/3. This variant also under predicts the boundary fluxes of the regional model by 1/6, which may be due to the mismatch of the regional and site-scale conductors and rock domains. Figures 5.5-1 and 5.5-2 present the exit locations and stream tubes for this variant, which are little different from those of the Base Case. This indicates that the exit locations and the flow paths are strongly influenced by the deterministic fracture zones. As discussed in Section 3.5.3, the occurence and extent of these zones is uncertain, but this uncertainty cannot be rigorously evaluated using the geostatistical algorithms in the current version of HYDRASTAR.

	Net Flux Through Subdomain (m <sup>3</sup> /s x 10 <sup>-3</sup> )						
Model Surface	Regional	Base Case	Variant 2	Variant 5			
		25 m Scale	50 m Scale	Deterministic			
West	13.7 (in)	4.92 (in)	6.66 (in)	2.00 (in)			
East	0.916 (in)	0.77 (in)	0.730 (in)	0.234 (in)			
South	1.81 (in)	0.846 (in)	0.489 (out)	0.477 (in)			
North	0.625 (in)	0.538 (in)	0.340 (in)	0.0919 (in)			
Bottom	0.374 (in)	1.03 (in)	1.11 (in)	0.677 (in)			
Тор	18.1 (out)	8.11 (out)	8.34 (out)	3.49 (out)			
Total Inflow	17.4	8.11	8.83	3.48			
Total Outflow	18.1	8.11	8.83	3.49			
Mass balance	-0.675	-0.0037	0.009	-0.010			
(In – Out)							

Table 5.5-3 Boundary Flux Consistency for Aberg Base Case, Variant 2, Variant 5and Regional Models.



Figure 5.5-1. Exit locations for Aberg 5 (deterministic). Results for 120 starting positions. (Äspö local coordinate system, scale in metres).



a) Plan view



b) Elevation view, from South



c) Elevation view, from East

Figure 5.5-2. Stream tubes for realisation number 1 of Aberg Variant 5 (deterministic). The y-positive axis of a) points in the direction of Aspö local North. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1x10^{-4}$ .

# 6 Discussion and Summary

The SKB SR 97 study is a comprehensive performance assessment illustrating the results for three hypothetical repositories in Sweden. This study addresses the hydrogeologic modelling of Aberg, one of the three SR 97 sites. The study uses HYDRASTAR, a stochastic continuum groundwater flow and transport modelling program developed by SKB. The application is relatively straightforward, with the majority of the model parameters and boundary conditions explicitly specified in Walker et al. (1997). This section of the report summarises the modelled cases and discusses the main results of the study in terms of statistics for travel time, F-ratio and canister flux. It also summarises the findings of the study with regard to model parameter uncertainty.

# 6.1 Input Data

Input data for the model is unmodified from that given by Walker et al. (1997b) except for the rescaling of hydraulic conductivities as suggested by Walker et al. (1997b). The SKB geostatistical analysis code INFERENS is used to infer a regularised variogram model based on the 3 m interpreted hydraulic conductivities taken from SICADA.

The boundary conditions for this model are constant head boundaries, derived from a deterministic, freshwater, regional scale model modified from that of Svensson (1997a). The overall flow pattern of the regional model is typical of coastal areas: topographically driven flow from the inland areas exiting to the coastal waters. The transfer of regional heads via constant head boundaries preserves this pattern in the site-scale model. Adjustment of the scaling of hydraulic conductivity to fine-tune the boundary flux mass balance is not pursued.

## 6.2 Base Case

The Base Case uses 100 realisations of the hydraulic conductivity field with 120 starting positions to evaluate the travel times, canister fluxes and F-ratios for the proposed repository. As discussed in Section 4.0, the median travel times and median canister fluxes of the Base Case appear to be stable with respect to the number of simulations and are reasonably consistent with the regional model fluxes. All statistics are calculated with respect to the common logarithm transforms of the travel times, canister fluxes, and F-ratios to facilitate summary and display.

For the Base Case, the boundary fluxes of the regional model and the site scale model appeared to be consistent with respect to orientation, but the site-scale model may tend to underpredict the regional fluxes by a factor of approximately 1/2 to 1/3. While this

broadly supports the validity of the nested modelling and the associated upscaling, the site scale boundary fluxes are calculated for a relatively small number of realisations.

The ensemble results taken over all realisations of all starting positions suggest the following statistics for the Base Case:

- Median travel time is 10 years, with an interquartile range from 3.4 years to 37 years.
- Median canister flux is  $1.8 \times 10^{-3}$  m/year, with an interquartile range from  $3.7 \times 10^{-4}$  m/year to  $7.8 \times 10^{-3}$  m/year.
- Median F-ratio is  $1.0 \times 10^5$  year/m, with an interquartile range from  $3.4 \times 10^4$  year/m to  $3.7 \times 10^5$  year/m.

The current version of HYDRASTAR is limited to homogeneous flow porosity over the entire domain. Consequently, the F-ratio is a simple multiple of the travel time, and the canister flux is inversely correlated to the travel time. The  $\log_{10}$  travel time and  $\log_{10}$  canister flux distributions are slightly skewed as a consequence of the relatively high hydraulic conductivity in the region south of Äspö. The model domain is only slightly restrictive, with 0.5% of the stream tubes failing to reach the model domain upper surface.

The flow paths and exit locations of the realisations are compatible with the overall pattern of flow at the site. The travel times are consistent with scoping calculations based on Darcy's law and the observed gradient. The results are also consistent with the site-scale model of Svensson (1997b) and on-site head observations.

Three individual realisations are examined briefly to illustrate the variability within and between realisations. Although the stream tubes and exit locations may shift dramatically from one realisation to the next, the medians of performance measures are relatively stable between realisations.

Three individual starting positions are examined over all 100 realisations to illustrate variability due to the differences in stream tube starting positions. As suspected, placing a canister in a host rock of relatively low hydraulic conductivity increases the median travel time. Several individual regions and starting positions were studied, revealing that some areas were less preferable with respect to travel time (e.g., rock blocks with relatively high measured conductivities, the upper repository level relative to the lower repository level).

# 6.3 Variant Cases

### 6.3.1 Boundary Conditions

This study uses a nested modelling approach, with a regional model providing the sitescale boundary conditions. This set of variants evaluates the uncertainties associated with calculating and transferring boundaries between the regional and site-scale models. Four methods for determining boundary conditions are compared using a single realisation of the hydraulic conductivity field for the site-scale model. The effect of these boundary conditions are evaluated by comparing the travel time, canister flux and F-ratio and boundary flux. The four methods for calculating and transferring boundaries between the regional and site-scale models include the following:

- 1.1 Use a regional model with a deterministic, effective hydraulic conductivity and freshwater conditions (i.e., a single realisation of the Base Case, as discussed in Section 4.1)
- 1.2 Use a regional model with a single stochastic realisation of hydraulic conductivity and the observed salinity. Convert the resulting boundary pressures and salinities to environmental freshwater heads.
- 1.3 Use a regional model with a single stochastic realisation of hydraulic conductivity and freshwater conditions.
- 1.4 Avoid the regional model entirely and use the observed water table/sea level and hydrostatic conditions directly in the site scale model as simplified boundary conditions.

Variants 1.1, 1.2 and 1.3 suggest that the model results were relatively insensitive to the approach to calculating and transferring the heads from a regional model. The three methods for transferring boundary conditions from the regional model give similar values for median travel time and canister fluxes. In contrast, the simplified boundary condition variants, Variants 1.4b and 1.4c, suggested that the results were very sensitive to the regional flow patterns created by the use of nested modelling. A possible extension of this variant would be to investigate the effects of using constant flux (Neuman) or third-type boundaries that would allow greater head variance in the domain. Such boundary conditions are beyond the current capabilities of HYDRASTAR, however.

### 6.3.2 Upscaling

Hydraulic conductivity is thought to be a scale dependent parameter, but current research debates the correct method for scaling field measurements of hydraulic conductivity for use in continuum modelling. The Base Case uses the upscaling approach proposed by Walker et al. (1997b) to determine the mean and variogram of log hydraulic conductivity at the 25 m grid scale. This upscaling variant examines the

self-consistency of the upscaling approach by changing the model calculation scale to a 50 m regular grid. This new grid scale requires a commensurate rescaling of the simulation parameters for the hydraulic conductivity field.

The simulations indicate that changing the model grid scale from 25 to 50 m reduces the variance while increasing the range of the variogram and increasing the mean of  $log_{10}$  hydraulic conductivity. Monte Carlo simulations with this coarser grid yield travel times, canister fluxes and boundary fluxes that weakly agree with the Base Case. Although the method appears to be approximately self-consistent with respect to the median performance measures at various grid scales, the reduced travel times, the increased canister fluxes and increased boundary fluxes collectively suggest that the upscaling method may increase the effective hydraulic conductivity of the domain. The coarser grid also reduces the variability of the performance measures, as is expected with the decrease in the input variance of  $log_{10}$  hydraulic conductivity.

### 6.3.3 Anisotropic Variogram

Site investigations at Äspö and at various other locations in Sweden suggest that the host rocks may exhibit hydraulic anisotropy, which the current version of HYDRASTAR (1.7.2) cannot directly incorporate. This variant addresses the possible hydraulic anisotropy of the host rocks using an anisotropic variogram of hydraulic conductivities to create a large-scale anisotropic effective hydraulic conductivity. The overall effect is to create rough ellipsoids of conductivity, with the long axes parallel to the suggested major axis of anisotropy (northwest-southeast).

Two cases are evaluated, the first using a variogram anistropy ratio of 1:2:1 in the Vertical:NW:NE directions. Consistent with the findings of Svensson (1997a), the flow pattern is changed, with stream tubes reorganised parallel to the major axis of anisotropy. The second case uses a variogram anisotropy ratio of 1:10:1, resulting in stream tubes that are strongly oriented in the NW-SE direction. However, both variants indicate that the median performance measures are only slightly different from the Base Case. This may be a consequence of the coarseness of the model grid, which forces a simplification of the anisotropy ratio. This results in hydraulic conductivity fields with limited vertical correlation. Therefore, the preferential flow paths only exist in the NW-SE direction. For both cases, the only apparent difference is an increase in the variance of the performance measures and a reorganisation of the stream tubes.

### 6.3.4 Conditional Simulation

The Base Case of this study (Section 4) uses unconditional geostatistical simulation to create the hydraulic conductivity fields, and includes fracture zones as deterministic zones of increased mean log<sub>10</sub> hydraulic conductivity. An alternative approach is to condition the fields on observed hydraulic conductivity measurements via conditional simulation, and to include fracture zones implicitly with ordinary kriging. No deterministic fracture zones can be included rigorously in HYDRASTAR conditional simulations because it is not possible in practice to include such detailed kriging neighbourhoods in HYDRASTAR 1.7.2. Two variants are considered. The first is

unconditional simulation without deterministic fracture zones, which evaluates the effect of removing the conductive features from the Base Case. The second is conditional simulation without fracture zones, to evaluate the effects of conditioning the simulations on the observed hydraulic conductivities.

These variants use a simplified geostatistical model, with a variogram fitted to all of the hydraulic conductivities of the 3 m packer test data within the site-scale model domain. Both the variance and the  $log_{10}$  hydraulic conductivity are increased relative to the Base Case rock mass (SRD) parameters. These increases can be attributed to the inclusion of the CD data in the data used in the INFERENS variogram analysis.

The unconditional simulation without fracture zones has a median travel time half an order of magnitude lower than the Base Case, and the travel paths show no organisation around fracture zones. The change in median travel time is a result of removing the deterministic fracture zones, pooling all the data and determining a new geostatistical model. Removing the fracture zones (SCD) also appears to reduce the variance of travel time, since only a single domain is encountered by any given stream tube. Including the conditioning data yields slightly shorter travel times than the unconditional case. This may be the effect of the conditioning data creating relatively conductive regions where the packer tests results reflect the occurrence of a fracture zone. However, the large scale of the fracture zones (as in the Base Case) is not captured by conditional ssimulation because large amounts of measurement data are required to completely describe the fracture zone geometry. With the limited amount of data and short correlation length, the continuity of the fracture zone cannot be reproduced.

#### 6.3.5 Deterministic Simulation

This variant is a simplified simulation of the site using a deterministic representation of the hydraulic conductivity field (i.e., the field has no random component and thus needs only one 'realisation'). This variant uses the empirical upscaling rule (Appendix C.2) to determine the effective conductivity,  $K_e$ , for each rock unit. If the nested modelling and upscaling are consistent, the boundary fluxes should be approximately the same for the regional model, the Base Case and this deterministic variant.

The median travel time and median canister flux are slightly higher than that of the Base Case, while the variances of both of these measures are dramatically reduced, as expected for a deterministic field. However, this variant under predicts both the Base Case boundary fluxes and the boundary fluxes of the regional model. Taken with Variant 2 (upscaling), this variant suggests that the upscaling approach is generally self-consistent but could be investigated further.

### 6.3.6 Comparison

Table 6.1 presents a summary of the medians and variances of the performance measures for the Base Case (in bold) and for Variants 2 through 5. Variant 1 was not included because only a single realisation was considered, and the mean and variance of the performance measures cannot be compared to the ensemble values from the other

variants. However, note that Variant 1 indicated that alternative methods for transferring boundary conditions had little impact on the performance measures. Variant 4.2, using conditional simulation, yields the shortest median travel time and greatest median canister flux. The anisotropic variogram case, Variant 3.1, yields the longest median travel time and lowest median canister flux.

Figures 6-1 and 6-2 present floating histograms of the log<sub>10</sub> travel time and log<sub>10</sub> canister flux, respectively, for the Base Case, and Variant Cases 2, 3.1, 4.2, and 5. Note that the variabilities of the performance measures are quite high for the Base Case, and that the variability between the variants is comparatively low. For example, the Base Case has an interquartile range from 3.4 years to 37 years, while the range of median travel times for the variants is from 3.2 years (Variant 4.2) to 12 years (Variant 3.1). Thus the variability of the Base Case due to parameter variability is greater than the variability of the cases studied to address uncertainty. Within the limitations of the variant cases studied, this suggests that Base Case has adequately characterised the Aberg hypothetical performance.

Performance Measure		Base Case	Variant 2 Upscaling to 50 m	Variant 3.1 Anisotropic Variogram	Variant 4.2 Conditional Simulation	Variant 5 Deterministic
Log <sub>10</sub> Travel time	Median	1.015	0.766	1.091	0.502	1.074
(years)	Variance	0.599	0.426	0.677	0.512	0.273
Log <sub>10</sub> Canister Flux (m/y)	Median	-2.736	-2.400	-2.803	-2.087	-2.672
	Variance	0.935	0.560	1.034	0.973	0.192
F-ratio (y/m)	Median	5.015	4.766	5.091	4.502	5.074
	Variance	0.599	0.426	0.677	0.512	0.273

 Table 6.1. Summary of Aberg flow modelling results.



Figure 6-1. Floating histograms of  $log_{10}$  travel time for Base Case, Variants 2, 3.1, 4.2 and 5, each normalised to the number of stream tubes with travel times less than 10,000 years. Results for 120 starting positions and a flow porosity of  $\varepsilon_f = 1 \times 10^{-4}$ .



Figure 6-2. Floating histograms of  $log_{10}$  canister flux for the Base Case, Variants 2, 3.1, 4.2 and 5, each normalised to the total number of stream tubes.

# 6.4 Possible Model Refinements

In several respects, the modelling could be improved within the current features of HYDRASTAR. These include the use of a denser grid to improve the representation of both the fracture zones and the variogram of hydraulic conductivity. This improved representation would allow a more rigorous examination of possible hydraulic anisotropy. The number of realisations may have to be increased to improve the stability of performance measures if the performance of individual starting positions is of interest.

Other model refinements are possible but are outside of the current features of HYDRASTAR. These include the development and use of alternative upscaling methods that would be more widely applicable and self-consistent. Nonparametric geostatistical simulation might allow a more realistic representation of the observed distribution of hydraulic conductivities. A stochastic representation of conductive features would allow a more rigorous evaluation of the fracture zone uncertainties. And finally, a variant case to investigate the effects of using constant flux (Neuman) or third-type boundaries is suggested to examine changes to the head variance within the domain.

# 6.5 Summary of Findings

The Base Case results suggest that the expected performance measures of the Aberg hypothetical repository are as follows:

- The median travel time is 10 years, with an interquartile range from 3.4 years to 37 years.
- The median canister flux is  $1.8 \times 10^{-3}$  m/year, with an interquartile range from  $3.7 \times 10^{4}$  m/year to  $7.8 \times 10^{-3}$  m/year.
- The median F-ratio is  $1.0 \times 10^5$  year/m, with an interquartile range from  $3.4 \times 10^4$  year/m to  $3.7 \times 10^5$  year/m.

The Base Case model is supported by the scoping calculations, previous modelling studies, and on-site observations. The variant cases suggest that the median travel time ranges from 3.2 to 12 years, the median canister flux ranges from 1.5 to 8.2 x  $10^{-3}$  m/year, and the median F ratio ranges from 0.32 to 1.2 x  $10^{-5}$  year/m. The variability of the Base Case due to parameter variability is greater than the variability of the cases studied to address uncertainty. Within the limitations of the variant cases studied, this suggests that Base Case has adequately characterised the Aberg hypothetical performance.

Other notable findings of this study can be summarised as follows:

• The canister flux appears to be inversely correlated to the travel time.

- The flow paths and exit locations are compatible with the pattern of flow at the site, and appear to be dominated by the deterministic fracture zones.
- The performance measures are relatively insensitive to alternative methods of incorporating the regional boundary conditions, but are very sensitive to the regional flow patterns.
- The upscaling method used in this study appears to be approximately self-consistent with regard to the medians of the performance measures.
- The performance measures are relatively insensitive to the anisotropic variogram, but this effect may be limited by the model grid density.
- The conditional and unconditional variants that rely on Moye's formula upscaling and a pooled data set of both rock mass and fracture zone data results in the shortest travel times and greatest canister fluxes.

# Acknowledgements

The authors of this report would like to acknowledge the support and guidance of Anders Ström and Jan-Olof Selroos of the Swedish Nuclear Fuel and Waste Management Company (SKB). This study has benefited enormously from the review comments of Johan Andersson and Sven Follin of Golder Grundteknik, and Ingvar Rhén, VBB VIAK. Raymond Munier of Scandia Consult and Urban Svensson of CFE contributed data, ideas and useful comments throughout this study. Lydia Biggs of DE&S produced a number of the illustrations in this report, and the final text has benefited enormously from the careful editing of Marcie Summerlin of DE&S.

At the end of a long study, it is tempting to list all of modelling team members as coauthors on the final report, but this would be a practical impossibility. The efforts of the following contributors are appreciated and are hereby acknowledged:

- Maria Lindgren and Hans Widén (Kemakta) implemented the structural model and assisted in setting up the HYDRASTAR model for this study.
- Niko Marsic (Kemakta) postprocessed the model output to provide the statistical summaries of results, and Lars Lovius (Hellström and Lovius Data) provided general support for the HYDRASTAR simulations and postprocessing of results.
- Björn Bergman (DE&S) performed the scoping calculations for travel time, and along with Cecilia Andersson (DE&S) assisted in preparing the preliminary sections of the report.
- Gregory Ruskauff (DE&S) assisted in the geostatistical analysis and helped review and summarise the study.

This study was funded by The Swedish Nuclear Fuel and Waste Management Company (SKB).

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# **APPENDIX A. Definition of Statistical Measures**

# A.1 Floating Histograms

This study generally uses binned histograms to display the frequency distributions of the performance measures. The bin width of such histograms is determined by the default algorithms of Statistica. Although the bin width is somewhat subjective, binned histograms do provide a relatively unprocessed image of the data. However, binned histograms are not well-suited to graphical comparisons (e.g. overlaying multiple binned histograms is confusing to the eye).

An alternative method of constructing a frequency distribution histogram is to use a floating histogram. Floating histograms are single curved line representations of the frequency of the data. Although floating histograms are smoothed representations of the data, they are more legible when superimposed for the comparison of multiple histograms.

Statistica (Appendix F) calculates smoothed histograms using a moving window as a filter passing over the ordered sequence of the data. For each data value centred in the window, the frequency is calculated as the fraction of the data falling within the window. The width of the window in Statistica is set to  $\pm \frac{1}{2}$  an order of magnitude around the data value in the centre of the window.

## A.2 Statistical Significance of the Comparison of Distributions

Section 5 makes a number of comparisons of variant cases versus the Base Case or versus other variants, concluding that the 'distributions are significantly different'. This statement of significance is quantitatively supported by a statistical comparison of the distributions, testing the null hypothesis:

H<sub>0</sub>: the distributions are the same

The significance of this test, or p-value, is the probability of rejecting  $H_0$  when it is in fact true (a so-called Type I error). Thus, a small p-value indicates that we can safely reject the hypothesis that the distributions are the same (Larsen and Marx, 1986). Because the distributions to be compared in this study are skewed, they are not suited to test statistics that assume normally (Gaussian) distributed data. This study therefore uses nonparametric (distribution-free) test statistics to compute the p-value of the above test. The Kolmogorov-Smirnov test (K-S) is a nonparametric test used to compare distributional shapes (i.e., skewness, variability, and location), as documented in the

Statistica manual. The p-value of a K-S test of  $H_0$  is computed for the various combinations of the Base and variant cases (Tables A-1, A-2, A-3, and A-4).

Note: When computing the p-value for the comparisons of  $log_{10}$  travel time distributions, times greater than the default maximum travel time of 10,000 years are deleted from the distributions prior to the comparison. The resulting K-S p-value therefore ignores the flow paths failing to exit the upper surface of the model.

Case	Base Case	Variant 2	Variant 3.1	Variant 3.2	Variant 4.1	Variant 4.2
Base Case	-	Reject (p<0.001)				
Variant 2	Reject (p<0.001)	-	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 3.1	Reject (p<0.001)	Reject (p<0.001)	-	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 3.2	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	-	Reject (p<0.001)	Reject (p<0.001)
Variant 4.1	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	-	Reject (p<0.001)
Variant 4.2	Reject (p<0.001)	-				

 Table A-1
 Test for Similarity of Travel Time Distributions (Kolmogorov-Smirnov 2-sample).

Table A-2Test for Similarity of Canister Flux Distributions (Kolmogorov-<br/>Smirnov 2-sample).

Case	Base Case	Variant 2	Variant 3.1	Variant 3.2	Variant 4.1	Variant 4.2
Base Case	-	Reject (p<0.001)	Reject (p<0.025)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 2	Reject (p<0.001)	-	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 3.1	Reject (p<0.025)	Reject (p<0.001)	-	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 3.2	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	-	Reject (p<0.001)	Reject (p<0.001)
Variant 4.1	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	-	Reject (p<0.001)
Variant 4.2	Reject (p<0.001)	-				

Case	Variant 1.1	Variant 1.2	Variant 1.3	Variant 1.4a	Variant 1.4b	Variant 1.4c
Variant 1.1	-	Accept (p>0.1)	Accept (p>0.1)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 1.2	Accept (p>0.1)	-	Accept (p>0.1)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 1.3	Accept (p>0.1)	Accept (p>0.1)	-	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 1.4a	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	-	Reject (p<0.005)	Reject (p<0.001)
Variant 1.4b	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.005)	-	Accept (p>0.1)
Variant 1.4c	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Accept (p>0.1)	-

Table A-3 Test for Similarity of Travel Time Distributions in Variant 1(Kolmogorov-Smirnov 2-sample test, for a single realisation).

 

 Table A-4
 Test for Similarity of Canister Flux Distributions (Kolmogorov-Smirnov 2-sample test, for a single realisation).

Case	Variant 1.1	Variant 1.2	Variant 1.3	Variant 1.4a	Variant 1.4b	Variant 1.4c
Variant 1.1	-	Accept (p>0.1)	Accept (p>0.1)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.005)
Variant 1.2	Accept (p>0.1)	-	Accept (p>0.1)	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.005)
Variant 1.3	Accept (p>0.1)	Accept (p>0.1)	-	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)
Variant 1.4a	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	-	Accept (p>0.1)	Accept (p>0.1)
Variant 1.4b	Reject (p<0.001)	Reject (p<0.001)	Reject (p<0.001)	Accept (p>0.1)	-	Accept (p>0.1)
Variant 1.4c	Reject (p<0.005)	Reject (p<0.005)	Reject (p<0.001)	Accept (p>0.1)	Accept (p>0.1)	-

# APPENDIX B. Supplemental Regional Simulations

### **B.1** Approach

This application of HYDRASTAR employs a nested modelling strategy, with the sitescale model taking its boundary conditions from a regional model of much greater extent. Because the area is adjacent to the brackish Baltic Sea, it is possible that saltwater intrusion of Baltic sea water may create density dependent effect. However, HYDRASTAR cannot incorporate these effects directly, and must adapt the regional model heads to freshwater equivalent conditions. Similarly, regional models of hydraulic conductivity are uncertain; some authors have suggested stochastic models on the regional scale, whereas others have suggested deterministic (Walker et al, 1997b).

This section of the report describes the regional boundary conditions and the methods used to transfer these conditions to the site-scale HYDRASTAR model. For the purpose of this modelling study, Urban Svensson of CFE was contracted to perform supplementary simulations using the Aberg regional model described in Svensson (1997a). The resulting pressures, salinities and fluxes were delivered on a 100 m grid for variants 1.1, 1.2 and 1.3, and then interpolated to the site scale model grid as described below. Variant 1.4 addressed the feasibility of using simplified boundary conditions. The variants to study the influence of the boundary conditions are as follows:

- 1.1 Deterministic, effective hydraulic conductivity and freshwater conditions (i.e., the Base Case discussed in Sections 4.1 and 4.2).
- 1.2 Regional model with a single stochastic realisation of hydraulic conductivity and the observed salinity. The resulting boundary pressures and salinities are converted to environmental freshwater heads.
- 1.3 Regional model with a single stochastic realisation of hydraulic conductivity and freshwater conditions.
- 1.4 Simplified boundary conditions obtained from estimated watertable using topography data and sea level.

## **B.2 Transferring Boundary Conditions from PHOENICS to HYDRASTAR**

The PHOENICS regional boundary condition values for each case were delivered in two files, one for the top surface and one for the other sides of the model. The files contain coordinates and the corresponding fluid pressures in PA. The values are given for a 100 m grid and need to be transferred to the 25 m block size used in the site scale model. The pressures at the vertical sides and the bottom are given in one file, and the pressures at the top are given in another. These data are processed for HYDRASTAR input as follows:

- 1. The files (e.g. Press and Pz0) are concatenated to one file.
- 2. The file is sorted for x, y, z letting the corresponding pressure value follow using e.g. Excel
- 3. The sorted file is processed using a MATLAB script, which:
  - reads the concatenated pressure file and a file with the local model coordinates,
  - interpolates the values to 25 m for each face, using 2D linear interpolation,
  - visualises the interpolated values, and
  - writes it to a file named hypac.out, in HYDRASTAR format.
- 4. The file is transferred to the SKB Convex for use.

The 2D interpolation of head values is the same approach used by similar nested modelling studies (Ward et al., 1987; Leake et al., 1998).

### **B.3 Environmental Head**

For Variant 1.2, the regional model includes the effects of salinity. This necessitates an additional step to transfer boundary heads to the site-scale model, since HYDRASTAR does not address salinity dependence. One method for converting from saline water head to freshwater head is to calculate the environmental head (or density adjusted head). The environmental head (Lusczynski, 1961) is calculated as:

$$H_{e} = \frac{P - \int_{Z_{0}}^{Z} (\rho - \rho_{0}) g \, dz}{\rho_{0} g}$$

where *P* is the pressure,  $\rho$  is the density of saline water,  $\rho_0$  is the density of fresh water, *z* is the vertical distance to the reference datum *z*<sub>0</sub>, and *g* is the acceleration of gravity.

### **B.4 Simplified Boundary Conditions**

Boundary conditions for Variant 1.4 were derived from topographic data (data delivery from Ragnar Ström, SKB). The files, SITE20\_4.DAT (elevation data in XYZ format – 20 m spacing), SITE20\_4.GRD (elevation data in SURFER grid format – 20 m spacing) and ASPOKUST.BNA (coastline), were received May 4, 1998. The topographic data were converted into head boundary conditions for the top of the model domain by interpolation of elevation data to 25 m grid, estimation of water table and conversion into HYDRASTAR format i.e. in PA. The interpolated topography is shown in Figure B.1. Mean sea level was used for area covered by the Baltic sea.

The estimation of the water table, W.T., was calculated by:

W.T. = 0.333Z - 0.39 (m)

constrained by W.T. greater or equal to zero.



Figure B.1. The topography and sea level at the modelling region.

Three approaches were tested for the lateral and bottom boundary conditions. Variant 1.4a uses topographic head on the top, depth dependent head on the vertical sides and hydrostatic head on the bottom. The resulting gradient ignores vertical gradients along

the model sides, allowing many stream tubes to exit the model's lateral boundaries, as shown in the pattern of exit locations shown in Figure B.2. This is thought to be an unrealistic representation, and is not pursued further.

In Variant 1.4b, no-flow boundary conditions were used on all sides except the top, where the same topographic boundary conditions is used as in Variant 1.4a. In Variant 1.4c, hydrostatic head was used on the vertical sides and no-flow condition on the bottom (Figure B.3). Approach 1.4b results in all of the stream tubes arriving at the model's upper surface. Approach 1.4c gives statistics more like the Base Case.



*Figure B.2. Exit locations in Variant 1.4a. Boundary conditions on the surface based on the topography and hydrostatic head on the vertical sides and bottom.* 



Figure B.3. Boundary conditions on the southern side forVariant 1.4c.

# **APPENDIX C. Supplemental Calculations**

### C.1 Inference of Anisotropic Variogram

HYDRASTAR requires a stochastic description of hydraulic conductivity at the model grid scale, including the expected value of hydraulic conductivity and its spatial variogram. This is complicated by the suggestion of Rhén et al. (1997) that the host rocks at Äspö exhibit hydraulic anisotropy – a feature that HYDRASTAR cannot directly include in its simulations. In addition, the upscaling method in HYDRASTAR and INFERENS is heuristic even for scalars, and was not developed to account for hydraulic anisotropy. However, for the purposes of SR 97, this study evaluates the effects of hydraulic anisotropy on the performance assessment.

Gutjahr et al. (1978) found that a large-scale hydraulic anisotropy can evolve from isotropic (scalar) point values of hydraulic conductivities with an anisotropic spatial variogram. That is, the anisotropic variogram of isotropic point hydraulic conductivities creates a large-scale anisotropic effective hydraulic conductivity. The following Sections describe an attempt to exploit this relationship and infer an anisotropy variogram for the Äspö site, following an approach similar to that of Neuman and Depner (1988).

#### C.1.1 Theory

Gutjahr et al. (1978) used a first-order, perturbation approach to determine that the three-dimensional statistically anisotropic effective conductivity can be expressed as:

$$K_{ii} = K_{g} \left[ 1 + \sigma^{2} \ln \kappa \left( \frac{1}{2} - g_{ii} \right) \right]$$
(C.1)

*i* = 1, 2, 3 (no sum on *i*)

Where:

$$g_{ii} = \int \int_{-\infty}^{\infty} \int \frac{k_i k_j}{k^2} \frac{\lambda_1 \lambda_2 \lambda_3 dk_2 dk_3}{\pi^2 (1+u^2)^2}$$
$$u^2 = \lambda_1^2 k_1^2 + \lambda_2^2 k_2^2 + \lambda_3^2 k_3^2$$

 $K_{ii}$  = the components of the anisotropic effective conductivity, K<sub>e</sub>

Ln*K* = natural logarithm of the point values of hydraulic conductivity (isotropic).

 $K_g$  = the geometric mean of K

 $\lambda_i$  = the integral scale of the variogram of ln*K* in direction i

 $k_i$  = the spectrum of ln*K* in direction i.

Also note that Gelhar and Axness (1983) suggested that equation C.1 could be extrapolated to larger values of  $\sigma_{lnK}$  using:

$$K_{ii} = K_g \exp\left[\sigma_{\ln K}^2 \left(\frac{1}{2} - g_{ii}\right)\right]$$
(C.2)

This solution suggests that, although  $\ln K$  is hydraulically isotropic, the anisotropic variogram of  $\ln K$  creates an effective hydraulic conductivity that is hydraulically anisotropic. Further, it suggests that the components of an anisotropic effective hydraulic conductivity,  $K_e$ , can be estimated from the mean and anisotropic variogram of  $\ln K$ .

At many sites, boreholes are subvertical and the horizontal spacing is such that only the vertical component of the variogram can be estimated using traditional geostatistical methods (Winberg, 1989; La Pointe 1994). In this situation, Hufschmied (1986) and Neuman and Depner (1988) suggested that, if one knew  $K_{ii}$  from interference tests and the vertical variogram and  $K_g$  from packer tests, it would be possible to estimate  $\lambda_i$ , the remaining components of the anisotropic variogram of LnK. Neuman and Depner began by rearranging equation C.2 to

$$g_{ii} = \frac{1}{2} + \left( \ln K_{ii} - K_g \right) \sigma_{\ln K}^{-2}$$
(C.3)

If, for example, we could estimate  $K_{ii}^*$  via interference tests, and estimate  $K_g^*$  and  $\sigma^{2*}_{lnK}$  via packer tests, we could therefore estimate  $g_{ii}^*$  via the above. However,  $g_{ii}^*$  also should be approximately equal to:

$$\hat{g}_{ii} = F_{ii} \sigma_{\ln K}^{-2} \tag{C.4}$$

Where  $F_{ii}$  found as a function of  $\hat{\lambda}_i$  via numerical integration. Neuman and Depner force this by requiring  $\hat{g}_{11} \equiv 1 - \hat{g}_{22} - \hat{g}_{33}$  and then minimising  $(\hat{g}_{22} - g_{22}^*)^2 + (\hat{g}_{33} - g_{33}^*)^2$  by repeated guesses of  $\hat{\lambda}_i$ .

#### C.1.2 Algorithm

In summary, the algorithm for estimating the components of the variogram is:

1. Estimate  $K_{ii}^{*}$  from cross-hole interference tests,  $K_{g}^{*}$  from packer tests, and  $\sigma_{lnK}^{2*}$  from packer tests, then calculate estimate  $g_{ii}^{*}$  by substituting into equation C.3. Note that we also constrain  $\sum g_{ij}^{*} = 1$  and force  $g_{11} = 1 - g_{22} - g_{33}$ .

- 2. Use the plots of  $g_{ii}$  versus  $\lambda_1/\lambda_2$ ,  $\lambda_1/\lambda_3$  from Gelhar and Axness (1983, figures 4a and b) to estimate  $\hat{\lambda}_i$  by successive guesses. Note that we solve for  $\lambda_2$  and  $\lambda_1$  using  $\lambda_3$  = vertical range determined from the observed point variogram estimates.
- 3. Apply the ratios  $\lambda_1/\lambda_2$ ,  $\lambda_1/\lambda_3$  to the upscaled isotropic variogram, previously determined via application of INFERENS (Walker et al., 1997).

The algorithm described above differs from that proposed by Neuman and Depner (1988) in several respects. The components of  $K_{ii}$  are taken from Rhén's analysis of multidirectional probehole tests, rather than a large scale, multidirectional test for anisotropy. Additionally, values for the numerical integration in (1) are taken from plots provided in Gelhar and Axness (1983, plots 4a and 4b), and thus the minimisation  $\Omega$  is found only approximately.

There are several reasonable concerns regarding the applicability of this algorithm to this problem. These include that the components  $K_{ii}$  are grossly estimated from probehole data, and that the integral scale  $\lambda$  is weakly defined by field data. Follin (1992) suggests that the solutions of Gutjahr et al (1978) may not be valid for fractured media since they assume that the point hydraulic conductivity is isotropic. The HYDRASTAR upscaling algorithm is heuristic, and does not specifically address anisotropy. We might speculate, for example, that the block conductivities should include both hydraulic and stochastic anisotropy, since the block scale lies between the two extremes of point and infinite scale (Indelman and Dagan, 1993).

### C.1.3 Application

Programs from GSLIB are used to analyse the 3 m data in the rock domain (i.e., deterministic fracture zones excluded) within the tunnel spiral (SRD3) to estimate the directional variograms. The median indicator variograms are used as robust-resistant estimators to augment the traditional variogram (Figures C.1, C.2 and C.3). The vertical direction is reasonably well defined with a practical range of around 80 m (correlation integral scale of 13 m). The other directions have virtually no pairs until 100 m separation, and are erratic beyond that distance (Figures C.4, C.5, and C.6).

Rhén et al. (1997) suggested an anisotropy of 100:1:10 for NW:NE:vertical hydraulic conductivity, which Svensson (1997a) applied using

10\*S : S/10 : S

where S = the hydraulic conductivity in SRD3 (at the appropriate scale).

The algorithm described in Section C.1.2 was used to infer variograms in the NW and NE directions, given the vertical variogram and Rhén's estimate. The results suggest that, at the 3 m scale, a suitable anisotropic variogram would be:

 $C_0$  (nugget) = 8.3, C1 (sill) = 7.2,

Practical Ranges: NW = 120 m, NE = 60 m, Vertical = 80 m

Note that, because the nugget is 50% of the total variance, the correlation integral scales are approximately 20, 10, and 15 m. This suggests that the zero nugget, isotropic exponential model fitted by INFERENS be converted to an anisotropic model using the anisotropy ratio 2:1:1.5 (for NW:NE:Vertical practical ranges). Preserving the vertical range, this yields practical ranges of approximately 129:65:97 m.

Note that the finite difference grid spacing is 25 m, and that this is larger than the shortest integral scale determined above (i.e., 65 m/3 < 25 m). Thus we should anticipate that the model grid is too coarse to implement this ratio (Bergman and Walker, 1998). This study consequently simplifies the ratio to 2:1:1, and uses 10:1:1 to assess the uncertainty. It is reasonable to expect that this will result in a one-dimensional large-scale effective anisotropy with the major axis in the NW direction.



*Figure C.1 Median Indicator variogram, vertical direction. 3 m Äspö data in rock domain.* 



Figure C.2 Median Indicator variogram, Northwest direction. 3 m Äspö data in rock domain.



Figure C.3 Median Indicator variogram, Northeast direction. 3 m Äspö data in rock domain.



Figure C.4 Variogram, Vertical direction. 3 m Äspö data in rock domain.



Figure C.5 Variogram, Northwest direction. 3 m Äspö data in rock domain.


Figure C.6 Variogram, Northeast direction. 3 m Äspö data in rock domain.

### C.2 Upscaling of Hydraulic Conductivity Model

#### C.2.1 Approach

The injection and pumping tests performed in the cored boreholes and tunnel probeholes are the principal source of hydraulic conductivity data. These tests were interpreted and the measurements reported for various depths, rock types, etc. as described by Rhén et al. (1997). The interpreted hydraulic conductivities for the 3 m packer tests were taken directly from the SKB SICADA database and analysed with the SKB geostatistical inference code INFERENS.

The scale of these measurements (as inferred from the packer length) is much different from the proposed model grid scale. As discussed in Walker et al. (1997b), hydraulic conductivity is a scale-dependent parameter, which requires that the measured hydraulic conductivities be upscaled to the finite difference grid scale of the model. Thus, HYDRASTAR requires that the geometric means of interpreted hydraulic conductivities found in SICADA must be rescaled. This study uses the scaling relationship provided in Rhén et al. (1997), which assumes that the geometric mean of hydraulic conductivity at the measurement scale, L<sub>m</sub>, may be adjusted for scale using the regression equation:

$$Log_{10}K_{gu} = Log_{10}K_{gm} + 0.782(Log_{10}L_u - Log_{10}L_m)$$

where:

 $K_g$  = geometric mean of hydraulic conductivity (m/s)

L = length scale (m), assumed equal to the packer interval.

The subscripts m and u refer to the measurement and upscaled values, respectively. Rhén et al. (1997) developed this empirical scaling relationship using the 3 m, 30 m, 100 m packer tests and full-length tests in the same cored boreholes.

#### C.2.2 Upscaling and Inference for 50 m Scale

This inference of spatial correlation models for Aberg site-scale hydraulic conductivity begins by dividing the domain into SRD1 through 5, the SCD. The elevation zones, SRD, and SCD are treated as step changes in the mean of log<sub>10</sub> conductivities, and a single variogram model is inferred for the entire domain (i.e., the same variogram for SRD and SCD). As discussed in Walker et al. (1997b), the correct approach to the upscaling of hydraulic conductivities to the numerical grid block is not known. As an interim approach, this study uses the Äspö scaling relationships of Rhén et al. (1997) to determine the geometric mean of hydraulic conductivity in each SRD and depth zone (Appendix C.2.1). The effect of upscaling on the variogram is determined by applying the Moye's formula-based regularisation algorithm and fitting a variogram–trend model via iterative generalised least squares estimation (IGLSE; see Neuman and Jacobsen,

1984) to the regularised data. The SKB program INFERENS, which includes the Moye's formula-based regularisation, automates the IGLSE fitting algorithm. Program restrictions of HYDRASTAR and INFERENS limit the geostatistical model to one variogram model for both domains. Because the majority of the 3 m packer tests fall in the SRDs and this data yields a clearer variogram, the geostatistical model will be developed from the interpreted hydraulic conductivities in the SRDs.

Walker et al. (1997b) explores the data and fits a model for the 24 m scale. This study merely repeats the INFERENS fitting using a 50 m regularisation scale, and applies the Äspö scale relationships to determine the geometric mean ( $K_g$ ) at the 50 m scale. The resulting experimental and model variograms are shown in Figure 5.2-1, and the upscaled  $K_g$  is presented in Table 5.2-1. The effect of the upscaling is to decrease the total variance of the experimental variogram and to increase the practical range.

### C.3 Scoping Calculation for Approximate Travel Times

The purpose of this section is to provide rough estimations of travel times to be used as check on the model results. It uses Darcy's law applied to a single travel path, with the hydraulic gradient roughly estimated from the observed watertable.

#### C.3.1 Approach

The approach is to apply Darcy's Law and use the hydraulic gradient  $(\nabla h)$  and hydraulic conductivity (K) from various reports. The apparent velocity  $(V_a)$  is found by:

Darcy's Law:  $V_a = K\nabla h$  (C.3.1)

The gradient is calculated by using the difference in watertable divided by the horizontal distances between the release and the exit locations.

Hydraulic gradient: 
$$\nabla h = \frac{h_{exit} - h_{start}}{Distance}$$
 (C.3.2)

The average particle velocity  $(V_{mean})$  is given by dividing the apparent velocity  $(V_a)$  by the porosity  $\rho$ .

Average particle velocity: 
$$V_{mean} = \frac{V_a}{\rho}$$
 (C.3.3)

The porosity is given a fixed value of  $\rho$ =1e-4 for all calculations. The travel times for the average particle is then given by

Travel times:  $travel time = \frac{Travel lenght}{V_{mean}}$  (C.3.4)

#### C.3.2 Application

The gradient is difficult to estimate due to the complexity of the flow pattern. For this scoping calculation, we assumed that the hydraulic head at the starting position could be estimated as the water table elevation immediately above the starting position of interest. The head at the exit location was taken to be sea level. For Aberg the watertable is taken from Figure 2-15, SKB 97-23.

The horizontal distances were measure at the map provided in Figure 2-17, SKB 97-23 with the block location found in SKB R-97-09. The values for the hydraulic conductivity used are taken from Table 2-8 and table 2-9 in SKB 97-23.

Three paths are considered:

- Path one: Start point in middle of Block 1 at -600 masl following a straight line trough SRD 1 up to surface with exit point 310 m north of start point. This represents a "slow" pathway.
- Path two: Start point in south part of block 4 at -600 masl following fracture NE-1a up to surface 270 m south of start point. This represents a "fast" pathway.
- Path three: Start point in middle part of block 1 at -500 masl south trough rock mass in 150 m to EW-1N, then within EW-1N east 400 m up to surface. This represents an "expected" pathway.

Path 1			
Hydraulic Gradient		0,01612903	
Rock mass	Travel length	Log10 K3	Log10 K24
SRD 1	675	-8.74	-8.03
Travel Times	K3	K24	
SRD 1	72.9 yr	14.2 yr	

Path 2			
Hydraulic Gradient		0,0037037	
Fracture	Travel length	Log10 K100	Log10 K24
NE-1	657	-5	-5.48
Travel Times	K100	K24	
NE-1	0.0563 yr	0.170 yr	

Path3			
Hydraulic Gradient	SRD 1		0.02
		EW-1N	0.005
Fracture		Travel length	Log10 K24
SRD 1		190	-8.03
EW-1N		500	-7.79
Total		690	
Travel Times		K24	
SRD 1		3.22787716	
EW-1N		19.5520992	
Total		22.8 yr	

# C.4 Error Analysis of Observed versus Model Simulated Heads

According to Anderson & Woessner (1992, p229), the acceptable level of head error (calibration target) for groundwater model is the sum of several independent errors, expressed as:

$$\sigma_T = \sigma_m + \sigma_i + \sigma_h + \sigma_t \tag{C.4.1}$$

where :

 $\sigma_{T}$  = the maximum acceptable total error of simulated vs. observed heads

 $\sigma_m$  = measurement error

 $\sigma_i$  = interpolation error

 $\sigma_h$  = Scale-up error arising from heterogeneity

 $\sigma_t$  = error arising from unmodelled transient effects

Rhén and Forsmark (1993) analyzed the Äspö piezometric data and reported that, for head measurements of 10 m or less, the total estimated measurement error in packed sections was  $\sigma_m \le 0.15$  m and  $\sigma_m \le 0.06$  m in open boreholes.

For this grid size, 25 m, the interpolation error would be the maximum difference in head (from the model simulated head at the node)that could be seen within a grid block. This would be the gradient times the maximum distance:

$$\sigma_i = J \cdot d_{\max} \tag{C.4.2}$$

where

J = gradient, which at Äspö is approximately 0.02 m/m

 $d_{\text{max}}$  is the distance from the block centre to the farthest corner in the block

$$d_{\text{max}} = \left[ (17.7)^2 + (12.5)^2 \right]^{\frac{1}{2}} = 21.7m$$

so that

 $\sigma_i = (0.02)(21.7) = 0.433m$ 

The error due to heterogeneity is difficult to quantify, since we should expect that each Monte Carlo realisation should be different from the next. Gelhar (1986) suggests that heterogeneity results in head variability that can be expressed as:

$$\sigma_h^2 = \frac{1}{3} J^2 \sigma_{\ln K}^2 \lambda^2 \qquad \text{in isotropic, 3-D fields} \qquad (C.4.3)$$

Where

 $\lambda$  = integral scale (isotropic), which at Äspö is approximately 32.3 m  $\sigma_{\log K}^2 = 2.7$ , which is approximately  $\sigma_{\ln K}^2 = 14.0$ 

so that

$$\sigma_h = \left\{ \frac{(0.02)^2 (14.0)(32.33)^2}{3} \right\}^{-1/2} = 1.40m$$

This error is large because the variance  $\sigma_{\ln K}^2$  is large. Although this expression for  $\sigma_h$  is thought to be valid only for  $\sigma_{\ln K}^2 \leq 1.0$  (Bakr, et al., 1978), it has been shown to be valid for much larger variances. (Gelhar, 1993). Note that, strictly speaking, equation C.4.3 was derived considering the unmodelled heterogeneity of a domain when the model is represented by a uniform effective conductivity. We attempt to model this heterogeneity in each Monte Carlo realisation, and thus this variance assumed to address the Monte Carlo variability as well.

Transient effects are also difficult to quantity. Rhén and Forsmark (1993) provide the max and min measured heads during 1990 & 1991. If we assume that the data is normally distributed and the range corresponds to a 95% confidence interval, then

$$\sigma_{heads} = \frac{\max - ave}{1.96}$$

so that the variance of the mean head is

$$\sigma_t = \sigma_{ave} = \frac{\sigma_{heads}}{\sqrt{n}}$$

The number of measurements, *n*, is not given in Rhén and Forsmark (1993), but should be on the order of 100. For the sections selected for examination, (max-ave) < 2.0 m, so that  $\sigma_{heads} = O(1)$  so that  $\sigma_t = O(10^{-1})$  and thus negligible relative to the other errors

In summary, the calibration target given in equation 1 is:

 $\sigma_T = 0.15 + 0.433 + 1.4 + (0.1) = 2.0 \text{ m} \text{ (in open boreholes)}$ 

and

 $\sigma_T = 0.06 + 0.433 + 1.4 + (0.1) = 1.9 \text{ m} \text{ (in packed sections)}$ 

# **APPENDIX D. Summary of Input Parameters**

Table D-1	Mechanisms and model parameters considered in this study when
	modelling groundwater flow at Aberg using HYDRASTAR.

Mechanism	HYDRASTAR model	parameter	Source
	Symbol (unit)	Description	
Topographically driven flow	-	Fracture zone and rock domain geometries	Based on the interpreted geologic structural model for the site, TR 97-06, Table A2-6
	T (m <sup>2</sup> /s)	Fracture zone transmissivities	Based on the interpreted geohydrological model for the site, TR 97-06, Tables A2-7 and A2-8. 100m interference tests rescaled as described in Section 3.0
	K (m/s)	Rock mass hydraulic conductivity	Based on the interpreted geohydrological model for the site (TR 97-06) and single- hole water injection tests on 3m scale. These tests are the basis for geostatistical analysis and are used directly in conditional simulation. Upscaling as described in Section 3.0. See Appendix C.
	$S_{s} (m^{-1})$	Specific storativity. Necessary for transient simulations.	Not used
	-	Top boundary condition	Constant head, as provided by Svensson. See Appendix B. Files: Pz0, Press
	-	Vertical/lower boundary conditions	Constant head, as provided by Svensson. See Appendix B. Files: Press
	-	BC Variant cases	<ul> <li>1.2 TR 97-09 as environmental head,</li> <li>Files: Psz0, Ps</li> <li>1.3 TR 97-09 as freshwater head, Files:</li> <li>Pz0, PressVert</li> <li>1.4: see Appendix B of this report</li> </ul>
	ε <sub>f</sub> (-)	Flow porosity Necessary for travel time calculation, but is poorly known in general	From TR 97-06, uniform throughout model at $\varepsilon_f=1\times10^{-4}$
Thermally and/or salinity driven flow	$\rho$ (kg/m <sup>3</sup> )	Groundwater density	Constant density.
Repository	Tunnel Layout		Two level (-500 and -600 masl) layout H, (for hydraulic structural model) from R 97-09 Figures 6-18 and 6-19. File: h_koord.xls
	Starting Positions		120 starting positions spread uniformly over layout H of R 97-09
	EDZ / Backfill K (m/s)		No / 10 <sup>-10</sup> m/s, based on SKB AR D-96- 011
Model Domain	-	Extent of model required to assess travel times	Premodelling study of Gylling et al., 1998.

## **APPENDIX E. Data Sources**

This appendix documents the data transfers from SKB archives that has been used as input to the calculations. These data include coordinates for fracture zones, deposition tunnels, observed heads and boundary conditions. These were taken directly from SKB SICADA database, as documented in this section. The data is summarised by type in Appendix D.

### E.1 For Coordinates and Previous Interpreted K Values

Date: 970324 18:02:21 Table(s): transient\_inj\_cd Columns :transient\_inj\_cd.idcode, transient\_inj\_cd.start\_date, transient\_inj\_cd.stop\_date, transient\_inj\_cd.seclen, transient\_inj\_cd.secup, transient\_inj\_cd.bc, transient\_inj\_cd.k\_steady\_state, transient\_inj\_cd.k\_injection, transient\_inj\_cd.k\_fall\_off, transient\_inj\_cd.k\_jacob, transient\_inj\_cd.k\_prel, transient\_inj\_cd.k, transient\_inj\_cd.skinfactor\_i, transient\_inj\_cd.skinfactor\_t, transient\_inj\_cd.spec\_cap, transient\_inj\_cd.goodness, transient\_inj\_cd.test\_date, transient\_inj\_cd.comment New Columns: midpoint Condition: Expr=secup+(seclow-secup)/2 Criteria: (transient\_inj\_cd.idcode ='KAS02' OR transient\_inj\_cd.idcode ='KAS03' OR transient\_inj\_cd.idcode ='KAS04' OR transient\_inj\_cd.idcode ='KAS05' OR transient\_inj\_cd.idcode ='KAS06' OR transient\_inj\_cd.idcode ='KAS07' OR transient\_inj\_cd.idcode ='KAS08' OR transient\_inj\_cd.idcode ='KLX01') AND transient\_inj\_cd.seclen =3 Result: 1300 rows written Filename: trans 1.csv Fileformat: CSV Coordinate system: Local Coordinate calculation column: midpoint

### E.2 For Rock/Conductor Codes and Rhén K Values

```
Date :970324 18:05:05
```

Tables :sic\_dba.transient\_inj\_cd

Columns :transient\_inj\_cd.idcode, transient\_inj\_cd.start\_date, transient\_inj\_cd.stop\_date, transient\_inj\_cd.seclen, transient\_inj\_cd.secup, transient\_inj\_cd.bc, transient\_inj\_cd.k\_steady\_state, transient\_inj\_cd.k\_injection, transient\_inj\_cd.k\_fall\_off, transient\_inj\_cd.k\_jacob, transient\_inj\_cd.k\_prel, transient\_inj\_cd.k, transient\_inj\_cd.skinfactor\_i, transient\_inj\_cd.skinfactor\_t, transient\_inj\_cd.spec\_cap, transient\_inj\_cd.goodness, transient\_inj\_cd.test\_date, transient\_inj\_cd.comment New Columns: midpoint Condition: Expr=secup+(seclow-secup)/2 Criteria: (transient\_inj\_cd.idcode ='KAS02' OR transient\_inj\_cd.idcode ='KAS03' OR transient\_inj\_cd.idcode ='KAS04' OR

```
transient_inj_cd.idcode ='KAS05' OR transient_inj_cd.idcode ='KAS06' OR
transient_inj_cd.idcode ='KAS07' OR transient_inj_cd.idcode ='KAS08' OR
transient_inj_cd.idcode ='KLX01') AND transient_inj_cd.seclen =3
Result: 1300 rows written
Filename: trans_r.csv
Fileformat: CSV
Coordinate system: RT
Coordinate calculation column: midpoint
Output to: File
_____
Date :970606 15:31:46
Table(s) :sic_dba.zone_model96
Columns :zone_model96.site, zone_model96.idcode,
      zone_model96.borehole, zone_model96.sub_secup,
      zone_model96.sub_seclow,
      zone_model96.zone_name, zone_model96.rocktype,
      zone_model96.k,
      zone_model96.k_source, zone_model96.qc_ok,
Criteria :1=1
Result : 1300 rows written to file.
Filename : /home/skbee/rhen_k.csv
File format : csv
```

### E.3 Structural Data

Coordinates for the fracture zones are based on the interpreted structural model given by Table A2-6 of Rhén et al., (1997). The hydraulic properties of the fracture zones and SRD's are from Walker et al. (1997b).

### E.4 Repository Lay-out

The layout of the repository is the two-level layout H, taken from Figures 6-18 and 6-19 of Munier et al (1997). The layout is described by tunnel endpoint coordinates in Excel spreadsheets, received directly from Raymond Munier of Scandia Consult. The file h\_koord.xls contains tunnel coordinates for a layout based on hydraulic structures and the file kapkoord.xls contains canister positions. The latter file was used to check that all the positions fall into the designed tunnels.

File	Main contents here	Date received	Source
h_koord.xls	Tunnel coordinates	April 16 1998	R. Munier, SCC
kapkoord.xls	Canister positions	April 16 1998	(and R 97-09)

### **E.5 Boundary Conditions**

Three sets of boundary conditions were obtained from Svensson (personal communication, 1998). The different sets correspond to the Base Case (deterministic regional realisation), Variant 1.2 (saline conditions as environmental head) and Variant 1.3 (single stochastic regional realisation). Variant 2 (increased block size) uses the same boundary conditions as the Base Case, but with less resolution in the interpolation. Variants 3, 4 and 5 use the same boundary conditions as the Base Case.

Case	Files	Main Contents	Date received	Source
Base	Press, Pz0	Pressure, coordinates	November 27 1997	Svensson, CFE
	Uvel, Vvel, Wvel	flux over the boundaries		
Variant 1.2	Ps, Psz0	Pressure, coordinates and salt concentration	March 23 1998	Svensson, CFE
	Uvel, Vvel, Wvel	flux over the boundaries		
Variant 1.3	PressVert, Pz0	Pressure, coordinates	March 25 1998	Svensson, CFE
	Uvel, Vvel, Wvel	flux over the boundaries		

### E.6 Location of HYDRASTAR Input Files

Files are located within the following directories on the SKB Convex or on the SKB SUN machines. The path to the input files and result files on Convex starts with:

/slow/s92/tmp-hyd/aberg

or on the SUN machines (e.g. sultan):

/net/s92/export/home/tmp-hyd/aberg

In each directory, there is a file with a short description of the performed simulations in addition to the necessary files for HYDRASTAR and result files:

README.txt Description of the problem

The necessary HYDRASTAR files and result files may be found at:

- abas/ Base Case with unconditional stochastic simulations, HYDRABOOT
- avar1.1/ Variant 1.1, Realisation 1 of the Base Case
- avar1.2/ Variant 1.2, Stochastic single realisation, saline case
- avar1.3/ Variant 1.3, Boundary conditions from stochastic regional realisation
- avar1.4a/ Variant 1.4a, Simplified boundary conditions
- avar 1.4b/ Variant 1.4b, Simplified boundary conditions
- avar 1.4c/ Variant 1.4c, Simplified boundary conditions
- avar2/ Variant 2, Coarse grid, stochastic, 100 realisations
- avar3a/ Variant 3.1, Anisotropic variogram (2:1:1), stochastic
- avar3b/ Variant 3.2, Anisotropic variogram (10:1:1), stochastic
- avar4/ Variant 4.2, Conditional stochastic continuum
- determ/ Variant 5, Deterministic calculations
- avar6/ Variant 4.1, Unconditional stochastic continum
- holes/ Borehole information

## **APPENDIX F. Additional Software Tools**

**INFERENS** (Norman, 1992b; Geier, 1993). INFERENS is a FORTRAN program developed by SKB that incorporates the HYDRASTAR regularisation algorithm and Universal Kriging via iterative generalised least squares estimation (IGLSE). It is necessary in this study because each of the sites in SR 97 divides the model domain into a series of fracture zones, rock masses and depth zones that represent stepwise changes in the hydraulic conductivity. HYDRASTAR represents this complex hydraulic conductivity field as a multivariate lognormal regionalised variable with local trends in log<sub>10</sub> hydraulic conductivity. A single variogram model is inferred for the entire domain (i.e., the same variogram for SRD, SCD, etc). Although not a restriction of HYDRASTAR itself, this study will consider the trends as constants within welldefined volumes in the domain (0 order trends in  $\log_{10} K_b$ ). This complex model of trend and spatial correlation violates the assumptions of ordinary least squares estimation (i.e., fitting trends by simple least squares regression). This study instead uses the more versatile IGLSE for universal kriging suggested by Neuman and Jacobsen (1984). INFERENS is an SKB computer program for geostatistical inference that automates the IGLSE fitting and data exploration (Norman, 1992b). INFERENS is unique in that includes the same regularisation algorithm as HYDRASTAR to upscale the data and apply universal kriging. Thus the resulting model of trends and variogram are compatible with the conditioning data and the chosen grid scale.

A program limitation prohibited using the crossvalidation option in INFERENS for this study. Alternative methods that met QA standards were not readily available during this study; therefore, crossvalidation was omitted.

**HYDRAVIS** (Hultman, 1997) HYDRAVIS is a graphical post-processor for HYDRASTAR, permitting users to view the repository layout, deterministic zones, hydraulic conductivities, stream tubes, and hydraulic heads. HYDRAVIS is an Advanced Visual Systems (AVS) system 5 application module developed by Cap Gemeni under contract to SKB. HYDRAVIS scans the HYDRASTAR input <casename>.hyd file and the output files for the required information, which is then displayed in a GUI format for the user. The system runs under Sun/OS, and requires a compatible version of AVS to be available. (AVS is a commercial software package for scientific visualisation on Windows NT and UNIX platforms).

**IGOR Pro** (WaveMetrics) IGOR Pro is a commercial Mac and MS/Windows package used in this study to produce exit location plots and special plots; e.g., for studying single realisations and single starting positions. IGOR Pro is an interactive programmable environment for data analysis and plotting. It handles large data sets (more than 100,000 points) and it includes a wide range of capabilities for analysis and graphing.

**MATLAB** (MathWorks) MATLAB is a commercial software package for numerical computation, visualisation and programming. It supplies a large number of high-level mathematical operations that are convenient for data analysis and visualisation. In this study, several MATLAB programs are used to interpolate between the regional and site-

scale modelling domains and to post-process HYDRASTAR results. These programs include the following:

#### GENERAL SCRIPTS FOR PRE-PROCESSING TO THE STATISTICA PACKAGE:

#### Path: 2149ac\matlab

- layerabc.m These files start up and run the GUI in MATLAB.
- layerfunc.m Reads the input data files and generates casename.nim. The definitions of

layers and end point areas are also made here as well as the definition of the string variable 'HomeDir'. This string must be adjusted to match the installation path of the MATLAB files.

- perfm.m Calculates the performance measures for the entire data file as well as for separate canisters (defined here) and layers or end point areas (depending on which model domain is being studied).
- perfmout.m Generates a text file called *casename\_s.txt* containing performance measures for the entire data file and the chosen canisters.
- a\_out.m Generates text files containing performance measures for the different layers of canisters in Aberg. They are given the names AbergX.txt where x is the number of the layer.

#### FOR INTERPOLATION AND VISUALISATION OF BOUNDARY CONDITIONS:

#### Path: 2149ac\aberg\bcplot

- Interpol2.m Interpolates the values from the regional model to  $$\ensuremath{\mathsf{HYDRASTAR}}$  format.
- rand\_a.m Creates a figure containing the boundary conditions of Aberg visualised as six sides of an opened box.
- boxplot.m Creates two figures containing the boundary conditions of Aberg visualised as boxes showed from different angles. This file is a subroutine used by rand a.m.
- cntrl\_1.m Function used by boxplot.m.
- cntrl\_2.m Function used by boxplot.m.

**Statistica** (StatSoft) Statistica is commercial MS/Windows software package that performs general statistical analysis of data. One of its strengths is a macro scripting language that allows users to automate a series of sorting, analysis and plotting operations. Under contract to SKB, Kemakta has developed scripts that translate

HYDRASTAR output and compute summary statistics of the simulation results. The first script, statistica.pl, is a Perl script that scans and extracts the raw HYDRASTAR travel time and canister flux files and organises them into a format for Statistica input. A second Perl script, endpoints.pl, extracts the exit locations from the HYDRASTAR travel path files. A Statistica Basic program, Hydrast\_.STB, is a Statistica Basic program that acts as a macro for the Statistica GUI. Optional outputs include tables of summary statistics, histograms, and box plots of canister fluxes, travel time and F-ratio. This study uses Statistica version 5.1 and the scripts documented in Boghammar and Marsic (1997). Marsic (1998) updated the script Hydrasta\_.STB for use in this study. Additional statistical post-processing was provided by MATLAB.

#### TRAZON

This program is a modification of HYDRASTAR 1.7.2 that helps identify the canister locations versus the deterministic zones. It reads the HYDRASTAR input <casename>.hyd file and compares the stream tube starting position versus the ZONE and XALFA definitions. If the starting position falls within a defined ZONE or XALFA, a comment is written to the logfile. This feature is intended to be included as an option in future versions of HYDRASTAR.

## **APPENDIX G. Base Case HYDRASTAR Input File**

```
#
  AVS
#-----
_____
#
    NAME: abas.hyd
    DESC: Base case HYDRASTAR LOCAL
#
AESPOE MODEL
  DATE: 980421
#
#
   USER: BJORN GYLLING, KEMAKTA
   VERSION: HS 1.7.1
#
#-----
_____
#
SYSTEM SAVE SCRATCH FILES
SYSTEM IGNORE ERRORS
#SYSTEM SKIP USER INTERFACE
#SYSTEM VERBOSE
BEGIN BLOCK COVARIANCE
# DETERMINISTIC YES
#SPHERIVAL MODEL
#SPHERIVAL ...

# VARIANCE 2.7

# RANGE 97.

VARIANCE 2.72

DANCE -32.33
BEGIN_DEF ANISOTROPY
          1.0
    KXX
    KXY
                0.0
            0.0
1.0
0.0
    KXZ
    KYY
    ΚYΖ
    ΚZΖ
                1.0
  END DEF
# RELATIVE_TOL 1.0E-8
RELATIVE_TOL 0.01
  NUM_ICOSAHEDRON 40
  NUM_LINES 0
                  0.0 0.0 0.0
  ORIGIN
               0.2
999.
  MUL FACTOR
  TRUNCATION
END_BLOCK
BEGIN BLOCK GEOM
# 25 METER BLOCK SCALE
  PHOENICS BC
#
#
  AXISLENGTH 2400. 2200. 1250.
NUMBER_OF_NODES 97 89 49
  BOUNDARY
            NAMMU
#
 BEGIN_DEF USER_SYSTEM
   XY_ROTATE 0.
   ZY_ROTATE 0.
TRANSLATE 950 6150 -1250
   SYSTEM RIGHT
 END_DEF
  BEGIN DEF WORLD_SYSTEM
    XY_ROTATE 0.0
ZY_ROTATE 0.0
    TRANSLATE 950 6150 -1250
  SYSTEM RIGHT
 END DEF
END BLOCK
#
```

```
BEGIN BLOCK KRGE NBH
  BEGIN DEF SECONDARY
    NORMAL 0. 0. 1.
    WIDTH 3000.0
OVERLAP 50.0
    MEASUREMENTS 16
  END DEF
END_BLOCK
BEGIN BLOCK KRIGE
 NUM ITERATIONS 60
  RESIDUAL_TOL
                 0.01
 METHOD
                 NR
 RESTART
                /skbtmp/2149/aberg
 PATH
END BLOCK
#
BEGIN BLOCK HYDROLOGY EQ
  NUM_ITERATIONS 16000
  RESIDUAL_TOL 1.0E-08
PRECOND DIAGONAL
  PRECOND
END_BLOCK
BEGIN BLOCK TRANSPORT
  TRANSPORT MODEL STREAM
  PLOT_TIMES
                  1
  BACK INTERPOL
                 NOBACKINT
  INTERVALS
                 FIXED
  DELIMITERS
                  1.0
                  10.0
                  100.0
                  1000.0
  END LIST
  LOGON
  TOLERANCE
                 0.2
 PRESENTATION 1.0
CELL SHIFTS 1024
 PLOTTING MOMENTS 1.0E4
# STREAM_TUBES 121
 STREAM_IULES 120
  VIEW
                 AT.T.
END_BLOCK
BEGIN BLOCK RESULT ESTIMATION
  PERIOD 1
   SAVE TRANSPORT TRANSPORT
END_BLOCK
BEGIN BLOCK PRESENTATION
   POST_PROCESSOR AVS
   PRESENT
                    ZDTR
                    ALL
   NUM REALIZATIONS
    1 2
   END LIST
   INTERACTIVE
MODEL_NAME
                    NO
                    FAA
   BEGIN DEF PSLICE
     GIN_DEF ...
NORMAL 0. (
IOF 105.
                    0. 0. -1.
      WIDTH
                    70.
      C THRESHOLD 0.
      V THRESHOLD 0.
```

END DEF END BLOCK BEGIN BLOCK TRENDS # REF DEPTH 40.0 ALFA -8.56 BETA 0.0 STORATIVITY 1.0 #EW-1N BEGIN DEF PLANE NAME P1 EQUATION -0.488965 0.8716844 -0.032849 -5636.181 TYPE UPPER END DEF BEGIN DEF PLANE NAME U1 EQUATION -0.488965 0.8716844 -0.032849 -5651.181 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME L1 EQUATION -0.488965 0.8716844 -0.032849 -5621.181 TYPE UPPER END DEF #EW-1S BEGIN DEF PLANE NAME P2 EQUATION -0.479232 0.8547282 -0.199440 -5472.543 TYPE UPPER END DEF BEGIN DEF PLANE NAME U2 -0.479232 0.8547282 -EOUATION 0.199440 -5487.543 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME L2 EQUATION -0.479232 0.8547282 -0.199440 -5457.543 TYPE UPPER END DEF #EW-3 BEGIN\_DEF PLANE NAME P3 EQUATION -0.199396 0.9611595 -0.190823 -6409.201 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U.3 EQUATION -0.199396 0.9611595 -0.190823 -6421.701 TYPE UPPER END\_DEF BEGIN\_DEF PLANE NAME L3 -0.199396 0.9611595 -EQUATION 0.190823 -6396.701 TYPE UPPER END DEF #EW-7 BEGIN DEF PLANE NAME P4

EQUATION -0.255724 0.156217 -5606.408 0.9540446 -TYPE UPPER END DEF BEGIN DEF PLANE NAME U4 EOUATION -0.255724 0.9540446 -0.156217 -5618.908 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L4 EQUATION -0.255724 0.9540446 -0.156217 -5593.908 TYPE UPPER END DEF #NE-1 BEGIN DEF PLANE NAME P5 -0.438044 EQUATION 0.8471511 0.3007530 -4905.346 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U5 EQUATION -0.438044 0.3007530 -4920.346 0.8471511 TYPE UPPER END DEF BEGIN DEF PLANE NAME L5 EQUATION -0.438044 0.3007530 -4890.346 0.8471511 TYPE UPPER END DEF #NE-2 BEGIN DEF PLANE NAME P6 EQUATION -0.788254 0.5727476 -0.224978 -2588.858 TYPE UPPER END DEF BEGIN DEF PLANE NAME U6 EQUATION -0.788254 0.5727476 -0.224978 -2601.358 TYPE UPPER END DEF BEGIN DEF PLANE NAME L6 EQUATION -0.788254 0.224978 -2576.358 0.5727476 -TYPE UPPER END\_DEF #NE-3 BEGIN DEF PLANE NAME P7 EQUATION -0.481357 0.8336931 0.2706488 -4462.135 TYPE UPPER END DEF BEGIN DEF PLANE NAME U7 -0.481357 EQUATION 0.8336931 0.2706488 -4487.135 TYPE UPPER END DEF

BEGIN DEF PLANE NAME L7 EOUATION -0.481357 0.8336931 0.2706488 -4437.135 TYPE UPPER END DEF #NE-4N BEGIN DEF PLANE NAME P8 -0.385083 EQUATION 0.8646853 -0.322537 -4794.608 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U8 -0.385083 EOUATION 0.8646853 -0.322537 -4814.608 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L8 EQUATION -0.385083 0.8646853 -0.322537 -4774.608 TYPE UPPER END DEF #NE-4S BEGIN DEF PLANE NAME P9 EQUATION -0.467000 0.204799 -4608.536 0.8602138 -TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U9 EOUATION -0.467000 0.8602138 -0.204799 -4628.536 TYPE UPPER END DEF BEGIN DEF PLANE NAME L9 EQUATION -0.467000 0.8602138 -0.204799 -4588.536 TYPE UPPER END\_DEF #NW-1 BEGIN DEF PLANE NAME P10 EQUATION 0.3677331 0.8660391 -3132.454 0.3387457 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME U10 EQUATION 0.3677331 0.3387457 0.8660391 -3144.954 TYPE UPPER END DEF BEGIN DEF PLANE NAME L10 EQUATION 0.3677331 0.3387457 0.8660391 -3119.954 TYPE UPPER END DEF #NNW-1BEGIN DEF PLANE NAME P11 EQUATION 0.9514486 0.0000000 -4312.293 0.3078076 TYPE UPPER

END DEF BEGIN DEF PLANE NAME U11 EQUATION 0.9514486 0.0000000 -4324.793 0.3078076 TYPE UPPER END DEF BEGIN DEF PLANE NAME L11 EQUATION 0.9514486 0.3078076 0.0000000 -4299.793 TYPE UPPER END DEF #NNW-2 BEGIN DEF PLANE NAME P12 EQUATION 0.9159572 0.4012761 0.0000000 -4958.393 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U12 EQUATION 0.9159572 0.0000000 -4970.893 0.4012761 TYPE UPPER END DEF BEGIN DEF PLANE NAME L12 0.9159572 EQUATION 0.4012761 0.0000000 -4945.893 TYPE UPPER END DEF #NNW-3 BEGIN DEF PLANE NAME P13 0.9995033 -0.0315147 EOUATION 0.0000000 -1921.132 TYPE UPPER END DEF BEGIN DEF PLANE NAME U13 EQUATION 0.9995033 -0.0315147 0.0000000 -1933.632 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L13 EQUATION 0.9995033 -0.0315147 0.0000000 -1908.632 TYPE UPPER END\_DEF #NNW-4 BEGIN DEF PLANE NAME P14 0.9882466 EQUATION 0.1255517 0.0872093 -3176.610 TYPE UPPER END DEF BEGIN DEF PLANE NAME U14 0.9882466 EQUATION 0.1255517 0.0872093 -3189.110 TYPE UPPER END DEF BEGIN DEF PLANE NAME L14

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EQUATION 0.9882466 0.0872093 -3164.110 0.1255517 TYPE UPPER END DEF #NNW - 5BEGIN DEF PLANE NAME P15 EQUATION 0 9987798 0.0493855 0.0000000 -2325.567 TYPE UPPER END DEF BEGIN DEF PLANE NAME U15 EQUATION 0.9987798 0.0493855 0.0000000 -2338.067 TYPE UPPER END DEF BEGIN DEF PLANE NAME L15 0.9987798 EQUATION 0.0493855 0.0000000 -2313.067 TYPE UPPER END DEF #NNW-6 BEGIN DEF PLANE NAME P16 EQUATION 0.9900987 0.1403732 0.0000000 -3266.708 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME U16 EQUATION 0.9900987 0.1403732 0.0000000 -3279.208 TYPE UPPER END DEF BEGIN DEF PLANE NAME L16 0.9900987 0.1403732 EQUATION 0.0000000 -3254.208 TYPE UPPER END DEF #NNW-7 BEGIN DEF PLANE NAME P17 EQUATION 0.9039969 0.4186277 0.0868357 -4915.147 TYPE UPPER END DEF BEGIN DEF PLANE NAME U17 EQUATION 0.9039969 0.4186277 0.0868357 -4927.647 TYPE UPPER END DEF BEGIN DEF PLANE NAME L17 EQUATION 0.9039969 0.4186277 0.0868357 -4902.647 TYPE UPPER END DEF #NNW-8 BEGIN DEF PLANE NAME P18 EQUATION 0.7071068 0.7071068 0.0000000 -6788.225 TYPE UPPER END DEF

BEGIN DEF PLANE NAME U18 EOUATION 0.7071068 0.7071068 0.0000000 -6800.725 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L18 EQUATION 0.7071068 0.7071068 0.0000000 -6777.725 TYPE UPPER END\_DEF #SFZ01 BEGIN DEF PLANE NAME P19 0.2026884 EQUATION 0.9792433 0.0000000 -12455.699 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME U19 EQUATION 0.2026884 0.9792433 0.0000000 -12468.199 TYPE UPPER END DEF BEGIN DEF PLANE NAME L19 EQUATION 0.2026884 0.0000000 -12443.199 0.9792433 TYPE UPPER END DEF #SFZ02 BEGIN\_DEF PLANE NAME P20 EOUATION 0.9672847 -0.2536935 0.0000000 4674.310 TYPE UPPER END DEF BEGIN DEF PLANE NAME U20 EQUATION 0.9672847 -0.2536935 0.0000000 4661.810 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME L20 EQUATION 0.9672847 -0.2536935 0.0000000 4688.810 TYPE UPPER END DEF #SFZ03a BEGIN\_DEF PLANE NAME P21 EQUATION 0.2539498 0.9672174 0.0000000 -7445.653 TYPE UPPER END DEF BEGIN DEF PLANE NAME U21 0.2539498 EOUATION 0.9672174 0.0000000 -7458.153 TYPE UPPER END\_DEF BEGIN\_DEF PLANE NAME L21 EOUATION 0.2539498 0.9672174 0.0000000 -7433.153 TYPE UPPER

END DEF #SFZ03b BEGIN DEF PLANE NAME P22 EQUATION 0.0455553 0.0000000 -8112.644 0.9989618 TYPE UPPER END DEF BEGIN DEF PLANE NAME  $\overline{U}22$ EQUATION 0.0455553 0.9989618 0.0000000 -8125.144 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L22 EQUATION 0.0455553 0.9989618 0.0000000 -8100.144 TYPE UPPER END\_DEF #SFZ03c BEGIN DEF PLANE NAME P23 EQUATION -0.006410 0.0000000 -8062.655 0.9999794 TYPE UPPER END\_DEF BEGIN\_DEF PLANE NAME U23 EQUATION -0.006410 0.9999794 0.0000000 -8075.155 TYPE UPPER END DEF BEGIN DEF PLANE NAME L23 -0.006410 EQUATION 0.9999794 0.0000000 -8050.155 TYPE UPPER END DEF #SFZ03d BEGIN DEF PLANE NAME P24 EQUATION EQUATION 0.0581538 0.0000000 -8222.178 0.9983076 TYPE UPPER END DEF BEGIN DEF PLANE NAME U24 EQUATION 0.0581538 0.9983076 0.0000000 -8234.678 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME L24 EQUATION 0.0581538 0.9983076 0.0000000 -8209.678 TYPE UPPER END DEF #SFZ03e BEGIN DEF PLANE NAME P25 EQUATION 0.0430223 0.0000000 -8172.187 0.9990741 TYPE UPPER END DEF BEGIN DEF PLANE NAME U25

EQUATION 0.0430223 0.0000000 -8184.687 0.9990741 TYPE UPPER END DEF BEGIN DEF PLANE NAME L25 EQUATION 0.0430223 0.9990741 0.0000000 -8159.687 TYPE UPPER END DEF #SFZ03f BEGIN\_DEF PLANE NAME P26 EQUATION -0.027657 0.9996175 0.0000000 -7766.554 TYPE UPPER END DEF BEGIN DEF PLANE NAME U26 EQUATION -0.027657 0.9996175 0.0000000 -7779.054 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME L26 EQUATION -0.027657 0.9996175 0.0000000 -7754.054 TYPE UPPER END DEF #SFZ04 BEGIN DEF PLANE NAME P27 EQUATION -0.548901 0.0000000 -5818.566 0.8358871 TYPE UPPER END DEF BEGIN DEF PLANE NAME U27 EQUATION -0.548901 0.8358871 0.0000000 -5831.066 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L27 EQUATION -0.548901 0.8358871 0.0000000 -5806.066 TYPE UPPER END DEF #SFZ05a BEGIN DEF PLANE NAME P28 EQUATION -0.398723 0.8007621 -0.446989 -4423.415 TYPE UPPER END DEF BEGIN DEF PLANE NAME U28 EQUATION -0.398723 0.8007621 -0.446989 -4435.915 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L28 EQUATION -0.398723 0.8007621 -0.446989 -4410.915 TYPE UPPER END DEF #SFZ05b

BEGIN DEF PLANE NAME P29 EOUATION -0.233401 0.8634220 -0.447242 -4675.218 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME U29 EQUATION -0.233401 0.8634220 -0.447242 -4687.718 TYPE UPPER END DEF BEGIN DEF PLANE NAME L29 -0.233401 0.8634220 -EOUATION 0.447242 -4662.718 TYPE UPPER END DEF #SFZ05c BEGIN\_DEF PLANE NAME P30 EQUATION -0.419466 0.7900307 -0.447101 -3832.040 TYPE UPPER END DEF BEGIN DEF PLANE NAME U30 EOUATION -0.419466 0.7900307 -0.447101 -3844.540 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME L30 -0.419466 0.7900307 -EQUATION 0.447101 -3819.540 TYPE UPPER END DEF #SFZ06a BEGIN DEF PLANE NAME P31 EQUATION -0.439634 0.8981770 0.0000000 -8231.319 TYPE UPPER END DEF BEGIN DEF PLANE NAME U31 0.8981770 EOUATION -0.439634 0.0000000 -8243.819 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L31 EQUATION -0.439634 0.8981770 0.0000000 -8218.819 TYPE UPPER END DEF #SFZ06b BEGIN DEF PLANE NAME P32 EQUATION -0.131607 0.9913019 0.0000000 -9067.080 TYPE UPPER END DEF BEGIN DEF PLANE NAME U32 EQUATION -0.131607 0.0000000 -9079.580 0.9913019 TYPE UPPER

END\_DEF BEGIN DEF PLANE NAME L32 EQUATION -0.131607 0.0000000 -9054.580 0.9913019 TYPE UPPER END DEF #SFZ06c BEGIN DEF PLANE NAME P33 EQUATION -0.127971 0.9917778 0.0000000 -9079.886 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME U33 EQUATION -0.127971 0.9917778 0.0000000 -9092.386 TYPE UPPER END\_DEF BEGIN\_DEF PLANE NAME L33 EQUATION -0.127971 0.0000000 -9067.386 0.9917778 TYPE UPPER END DEF #SFZ07a BEGIN\_DEF PLANE NAME P34 0.7482103 EQUATION -0.663461 0.0000000 -4272.753 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U34 EOUATION -0.663461 0.7482103 0.0000000 -4285.253 TYPE UPPER END DEF BEGIN DEF PLANE NAME L34 EQUATION -0.663461 0.0000000 -4260.253 EQUATION 0.7482103 TYPE UPPER END DEF #SFZ07b BEGIN\_DEF PLANE NAME P35 EQUATION -0.667030 0.7450302 0.0000000 -4257.660 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U35 -0.667030 0.7450302 EOUATION 0.0000000 -4270.160 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L35 EQUATION -0.667030 0.7450302 0.0000000 -4245.160 TYPE UPPER END DEF #SFZ10a BEGIN DEF PLANE NAME P36

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EQUATION -0.988371 0.1520572 0.0000000 2447.360 TYPE UPPER END DEF BEGIN DEF PLANE NAME U36 EQUATION -0.988371 0.1520572 0.0000000 2434.860 TYPE UPPER END\_DEF BEGIN\_DEF PLANE NAME L36 -0.988371 EQUATION 0.1520572 0.0000000 2459.860 TYPE UPPER END DEF #SFZ10b BEGIN DEF PLANE NAME P37 -0.965653 EQUATION 0.2598344 0.0000000 1498.702 TYPE UPPER END DEF BEGIN DEF PLANE NAME  $\overline{U}37$ EQUATION -0.965653 0.2598344 0.0000000 1486.202 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L37 -0.965653 EQUATION 0.2598344 0.000000 1511.202 TYPE UPPER END DEF #SFZ11 BEGIN DEF PLANE NAME P38 EQUATION 0.1978365 0.0000000 -7540.771 0.9802350 TYPE UPPER END DEF BEGIN DEF PLANE NAME U38 EQUATION 0.1978365 0.9802350 0.0000000 -7553.271 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L38 EQUATION 0.1978365 0.0000000 -7528.271 0.9802350 TYPE UPPER END\_DEF #SF713a BEGIN DEF PLANE NAME P39 EQUATION 0.4472136 0.8944272 0.0000000 -8152.704 TYPE UPPER END DEF BEGIN DEF PLANE NAME U39 EQUATION 0.4472136 0.8944272 0.0000000 -8165.204 TYPE UPPER END DEF

BEGIN DEF PLANE NAME L39 EQUATION 0.4472136 0.8944272 0.0000000 -8140.204 TYPE UPPER END DEF #SFZ13b BEGIN DEF PLANE NAME P40 EQUATION 0.2782189 0.9605177 0.0000000 -8506.609 TYPE UPPER END\_DEF BEGIN DEF PLANE NAME U40 EQUATION 0.2782189 0.9605177 0.0000000 -8519.109 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME L40 EQUATION 0.2782189 0.9605177 0.0000000 -8494.109 TYPE UPPER END DEF #SFZ14a BEGIN DEF PLANE NAME P41 -0.990023 EQUATION 0.1409022 0.0000000 -23.416 TYPE UPPER END\_DEF BEGIN\_DEF PLANE NAME U41 EOUATION -0.990023 0.1409022 0.0000000 -35.916 TYPE UPPER END DEF BEGIN DEF PLANE NAME L41 -0.990023 EQUATION 0.1409022 0.0000000 -10.916 TYPE UPPER END DEF #SFZ14b BEGIN DEF PLANE NAME P42 EQUATION -0.978468 0.2063957 0.0000000 -550.847 TYPE UPPER END DEF BEGIN\_DEF PLANE NAME U42 EQUATION -0.978468 0.2063957 0.0000000 -563.347 TYPE UPPER END DEF BEGIN DEF PLANE NAME L42 -0.978468 EOUATION 0.2063957 0.0000000 -538.347 TYPE UPPER END DEF #SFZ15 BEGIN\_DEF PLANE NAME P43 EOUATION -0.991411 0.1307767 1029.536 0.0000000 TYPE UPPER

END\_DEF BEGIN DEF PLANE NAME U43 EOUATION -0.991411 0.1307767 1017.036 0.0000000 TYPE UPPER END DEF BEGIN DEF PLANE NAME L43 -0.991411 0.1307767 EOUATION 0.0000000 1042.036 TYPE UPPER END DEF #FixNNW5 BEGIN DEF PLANE NAME F1 0.0000000 -1.0000000 EQUATION 0.0000000 7394.100 TYPE UPPER END\_DEF #FixNNW3N BEGIN DEF PLANE NAME E2 0.0000000 -1.0000000 EOUATION 0.0000000 7025.400 TYPE UPPER END DEF #FixNNW3S BEGIN DEF PLANE NAME F3 EQUATION 0.0000000 -1.0000000 0.000000 6812.900 TYPE UPPER END DEF #Fix NNW-8 BEGIN DEF PLANE NAME A1 EQUATION 0.0000000 0.000000 1.0000000 300.000 TYPE UPPER END DEF #Fix NNW-8 BEGIN DEF PLANE NAME A2 EQUATION 0.0000000 0.0000000 1.0000000 700.000 TYPE UPPER END DEF #Fix EW-5 BEGIN DEF PLANE NAME Q1 0.0000000 1.0000000 EQUATION 0.0000000 -7352.500 TYPE UPPER END\_DEF #Fix EW-5 BEGIN DEF PLANE NAME Q2 -1.000000 EOUATION 0.0000000 0.0000000 2265.000 TYPE UPPER END DEF #Fix EW-5 BEGIN\_DEF PLANE NAME Q3 EOUATION 0.0000000 1.0000000 0.0000000 -7277.500 TYPE UPPER END DEF #Fix EW-5 BEGIN DEF PLANE NAME 04

-1.000000 EQUATION 0.000000 0.0000000 2115.000 TYPE UPPER END DEF #Fix EW-5 BEGIN DEF PLANE NAME Q5 EQUATION 0.0000000 -0.0000000 -387.500 1.000000 TYPE UPPER END DEF #Fix EW-5 BEGIN\_DEF PLANE NAME Q6 EQUATION 0.0000000 0.0000000 -1.000000 -312.500 TYPE UPPER END DEF #Fix SFZ07a&b BEGIN DEF PLANE NAME X07 0.7466274 EQUATION 0.6652425 0.0000000 -3157.360 TYPE UPPER END DEF #Fix SFZ03b&c BEGIN DEF PLANE NAME X03 EQUATION 0.9998083 -0.0195816 0.0000000 -961.758 TYPE UPPER END DEF #Fix SFZ07c&d BEGIN DEF PLANE NAME X04 EQUATION 0.9996650 -0.0258815 0.0000000 -2469.974 TYPE UPPER END DEF #EW-1N BEGIN DEF ZONE NAME Z1 ALFA -7.79 BETA 0.0 STORATIVITY 1.0 PLANE U1 P\_TYPE UPPER PLANE L1 P TYPE LOWER PLANE P23 P TYPE UPPER PLANE P41 P TYPE UPPER TEST POINT 2002.87 7585.23 -109.13 END DEF #EW-1S BEGIN\_DEF ZONE NAME Z44 ALFA -6.62 BETA 0.0 STORATIVITY 1.0 PLANE U2 P TYPE UPPER PLANE L2 P TYPE LOWER PLANE P23 P TYPE UPPER PLANE P36 P TYPE LOWER PLANE P35 P TYPE UPPER TEST POINT 3124.00 7932.00 -905.00 END DEF #EW-1S BEGIN DEF ZONE

NAME Z45 ALFA -6.62 BETA 0.0 STORATIVITY 1.0 PLANE U2 P TYPE UPPER PLANE L2 P\_TYPE LOWER PLANE P35 P TYPE LOWER PLANE P41 P TYPE UPPER TEST\_POINT 1321.00 7008.00 -517.00 END DEF #EW-3 BEGIN DEF ZONE NAME Z3 ALFA -6.50 BETA 0.0 STORATIVITY 1.0 PLANE U3 P\_TYPE UPPER PLANE L3 P TYPE LOWER PLANE P5 P TYPE LOWER PLANE P41 P TYPE UPPER TEST POINT 2167.80 7082.03 -180.73 END DEF #EW-7 BEGIN DEF ZONE NAME Z4 ALFA -6.05 BETA 0.0 STORATIVITY 1.0 PLANE U4 P TYPE UPPER PLANE L4 P TYPE LOWER PLANE P8 P TYPE UPPER PLANE P36 P TYPE LOWER TEST POINT 2189.17 6450.60 -77.27 END DEF #NE-1 BEGIN\_DEF ZONE NAME  $\overline{Z}47$ ALFA -5.48 BETA 0.0 STORATIVITY 1.0 PLANE U5 P TYPE UPPER PLANE L5 P TYPE LOWER PLANE P41 P TYPE LOWER PLANE P35 P TYPE UPPER 640.00 6205.00 -234.00 TEST POINT END DEF #NE-1 BEGIN DEF ZONE NAME Z48 ALFA -5.48 BETA 0.0 STORATIVITY 1.0 PLANE U5 P\_TYPE UPPER PLANE L5 P TYPE LOWER PLANE P41 P TYPE UPPER PLANE P36

P TYPE LOWER PLANE P23 P TYPE UPPER PLANE P2 P\_TYPE UPPER TEST POINT 2542.00 7347.00 -682.00 END DEF #NE-2BEGIN DEF ZONE NAME Z6 ALFA -8.27 BETA 0.0 STORATIVITY 1.0 PLANE U6 P TYPE UPPER PLANE L6 P TYPE LOWER PLANE P2 P TYPE UPPER PLANE P5 P\_TYPE LOWER PLANE P3 P\_TYPE LOWER TEST POINT 2036.00 7276.40 -116.47 END DEF #NE-3 BEGIN DEF ZONE NAME Z7 ALFA -5.72 BETA 0.0 STORATIVITY 1.0 PLANE U7 P TYPE UPPER PLANE L7 P\_TYPE LOWER PLANE P38 P TYPE UPPER PLANE P35 P\_TYPE UPPER PLANE P29 P TYPE LOWER TEST POINT 2107.18 6593.47 -75.68 END DEF #NE-4NBEGIN DEF ZONE NAME Z8 ALFA -6.61 BETA 0.0 STORATIVITY 1.0 PLANE U8 P TYPE UPPER PLANE L8 P TYPE LOWER PLANE P38 P TYPE UPPER PLANE P36 P\_TYPE LOWER PLANE P29 P TYPE LOWER TEST POINT 2171.57 6484.10 -74.83 END DEF #NE-4S BEGIN DEF ZONE NAME Z9 ALFA -6.61 BETA 0.0 STORATIVITY 1.0 PLANE U9 P TYPE UPPER PLANE L9 P TYPE LOWER PLANE P8 P TYPE UPPER PLANE P29 P TYPE LOWER

TEST POINT -109.00 5066.00 -975.00 END DEF #NW-1 BEGIN DEF ZONE NAME  $\overline{Z}10$ ALFA -8.65 BETA 0.0 STORATIVITY 1.0 PLANE U10 P TYPE UPPER PLANE L10 P TYPE LOWER PLANE P1 P TYPE LOWER PLANE P23 P TYPE UPPER PLANE P41 P TYPE UPPER TEST POINT 1549.20 7775.60 -82.20 END DEF #NNW-1 BEGIN\_DEF ZONE NAME Z11 ALFA -6.84 BETA 0.0 STORATIVITY 1.0 PLANE U11 P TYPE UPPER PLANE L11 P TYPE LOWER PLANE P3 P TYPE LOWER PLANE P2 P\_TYPE UPPER TEST\_POINT 2176.87 7280.90 -666.67 END DEF #NNW-2 BEGIN DEF ZONE NAME Z12 ALFA -6.13 BETA 0.0 STORATIVITY 1.0 PLANE U12 P TYPE UPPER PLANE L12 P TYPE LOWER PLANE P5 P TYPE LOWER PLANE P2 P TYPE UPPER TEST POINT 2245.00 7232.10 -666.67 END\_DEF #NNW-3 BEGIN DEF ZONE NAME Z13 ALFA -6.79 BETA 0.0 STORATIVITY 1.0 PLANE U13 P TYPE UPPER PLANE L13 P TYPE LOWER PLANE F2 P TYPE LOWER PLANE F3 P TYPE UPPER TEST POINT 2139.13 6883.73 -666.67 END DEF #NNW-4 BEGIN\_DEF ZONE NAME Z14 ALFA -5.71 BETA 0.0 STORATIVITY 1.0 PLANE U14

P TYPE UPPER PLANE L14 P TYPE LOWER PLANE P5 P\_TYPE LOWER PLANE P2 P TYPE UPPER TEST POINT 2300.83 7291.93 -145.57 END DEF #NNW-5 BEGIN DEF ZONE NAME Z15 ALFA -7.58 BETA 0.0 STORATIVITY 1.0 PLANE U15 P TYPE UPPER PLANE L15 P TYPE LOWER PLANE P8 P TYPE LOWER PLANE F1 P\_TYPE LOWER TEST POINT 2001.47 6612.10 -666.67 END DEF #NNW-6 BEGIN DEF ZONE NAME Z55 ALFA -6.79 BETA 0.0 STORATIVITY 1.0 PLANE U16 P TYPE UPPER PLANE L16 P\_TYPE LOWER PLANE P8 P TYPE LOWER PLANE P4 P\_TYPE UPPER 2410.00 6290.00 -1000.00 TEST POINT END DEF #NNW-6 BEGIN DEF ZONE NAME Z56 ALFA -6.79 BETA 0.0 STORATIVITY 1.0 PLANE U16 P TYPE UPPER PLANE L16 P TYPE LOWER PLANE P5 P TYPE UPPER PLANE P2 P TYPE UPPER PLANE P4 P\_TYPE LOWER TEST\_POINT 2348.70 6705.43 -666.67 END DEF #NNW-7 BEGIN DEF ZONE NAME Z17 ALFA -7.20 BETA 0.0 STORATIVITY 1.0 PLANE U17 P TYPE UPPER PLANE L17 P TYPE LOWER PLANE P3 P TYPE LOWER PLANE P2 P TYPE UPPER TEST POINT 2059.33 7306.90 -61.67 END DEF

#NNW-8 BEGIN DEF ZONE NAME Z18 ALFA -6.88 BETA 0.0 STORATIVITY 1.0 PLANE U18 P TYPE UPPER PLANE L18 P TYPE LOWER PLANE P1 P TYPE LOWER PLANE P23 P TYPE UPPER PLANE A1 P TYPE UPPER PLANE A2 P TYPE LOWER TEST POINT 1866.67 7733.33 -433.33 END DEF #SFZ01 #BEGIN\_DEF ZONE #NAME Z19 #ALFA -7.41 #BETA 0.0 #STORATIVITY 1.0 #PLANE U19 #P TYPE UPPER #PLANE L19 #P TYPE LOWER #TEST POINT 4636.67 11760.00 -500.00 #END DEF #SFZ02 BEGIN\_DEF ZONE NAME Z20 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U20 P TYPE UPPER PLANE L20 P TYPE LOWER TEST POINT -3125.00 6510.00 -500.00 END DEF #SFZ03a #BEGIN DEF ZONE #NAME Z21 #ALFA -7.41 #BETA 0.0 #STORATIVITY 1.0 #PLANE U21 **#**P\_TYPE UPPER #PLANE L21 #P TYPE LOWER #PLANE P22 #P TYPE LOWER #TEST\_POINT -2680.00 8401.67 -500.00 #END DEF #SFZ03b BEGIN DEF ZONE NAME Z22 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U22 P TYPE UPPER PLANE L22 P TYPE LOWER PLANE P21 P\_TYPE LOWER PLANE X03 P TYPE UPPER TEST POINT -415.00 8140.00 -975.00 END DEF #SFZ03c

BEGIN DEF ZONE NAME Z23 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U23 P TYPE UPPER PLANE L23 P TYPE LOWER PLANE X03 P TYPE LOWER PLANE X04 P\_TYPE UPPER TEST POINT 1900.00 8075.00 -975.00 END DEF #SFZ03d BEGIN DEF ZONE NAME Z24 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U24 P TYPE UPPER PLANE L24 P TYPE LOWER PLANE X04 P TYPE LOWER PLANE P25 P TYPE LOWER TEST POINT 3195.00 8050.00 -975.00 END DEF #SFZ03e #BEGIN DEF ZONE  $\#NAME \overline{Z}25$ #ALFA -7.41 #BETA 0.0 **#STORATIVITY 1.0** #PLANE U25 #P TYPE UPPER #PLANE L25 #P TYPE LOWER #PLANE P24 #P TYPE LOWER #PLANE P26 #P TYPE LOWER #TEST POINT 5103.33 7960.00 -500.00 #END DEF #SFZ03f #BEGIN\_DEF ZONE #NAME Z26 #ALFA -7.41 #BETA 0.0 **#STORATIVITY 1.0** #PLANE U26 #P TYPE UPPER #PLANE L26 **#**P\_TYPE LOWER #PLANE P25 #P TYPE LOWER 7486.67 7976.67 -500.00 #TEST\_POINT #END DEF #SFZ04 BEGIN DEF ZONE NAME Z27 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U27 P TYPE UPPER PLANE L27 P TYPE LOWER PLANE P41 P TYPE LOWER TEST\_POINT -1016.67 6293.33 -500.00 END DEF

#SFZ05a BEGIN DEF ZONE NAME Z28 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U28 P TYPE UPPER PLANE L28 P TYPE LOWER PLANE P20 P TYPE LOWER PLANE P29 P TYPE UPPER TEST POINT -1978.67 4259.67 -500.00 END DEF #SFZ05b BEGIN DEF ZONE NAME Z29 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U29 P TYPE UPPER PLANE L29 P TYPE LOWER PLANE P28 P TYPE UPPER PLANE P30 P TYPE LOWER TEST POINT 1348.67 5520.33 -500.00 END DEF #SFZ05c BEGIN DEF ZONE NAME Z30 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U30 P TYPE UPPER PLANE L30 P TYPE LOWER PLANE P29 P TYPE LOWER PLANE P26 P TYPE UPPER 4705.67 7066.00 -500.00 TEST POINT END DEF #SFZ06a BEGIN DEF ZONE NAME Z31 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U31 P TYPE UPPER PLANE L31 P TYPE LOWER PLANE P21 P\_TYPE LOWER PLANE P32 P TYPE UPPER TEST POINT -683.33 8830.00 -500.00 END DEF #SFZ06b BEGIN DEF ZONE NAME Z32 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U32 P TYPE UPPER PLANE L32 P TYPE LOWER PLANE P31

P TYPE UPPER PLANE P33 P TYPE UPPER TEST POINT 1506.67 9346.67 -500.00 END\_DEF #SFZ06c BEGIN DEF ZONE NAME Z33 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U33 P\_TYPE UPPER PLANE L33 P TYPE LOWER PLANE P32 P TYPE UPPER 6315.00 9970.00 -500.00 TEST POINT END DEF #SFZ07a BEGIN DEF ZONE NAME Z34 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U34 P TYPE UPPER PLANE L34 P TYPE LOWER PLANE X07 P TYPE UPPER TEST POINT -2025.00 3915.00 -975.00 END DEF #SFZ07b BEGIN\_DEF ZONE NAME Z35 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U35 P TYPE UPPER PLANE L35 P TYPE LOWER PLANE X07 P TYPE LOWER PLANE P41 P\_TYPE LOWER 212.50 5905.00 -975.00 TEST\_POINT END DEF #SFZ10a BEGIN DEF ZONE NAME Z36 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U36 P\_TYPE UPPER PLANE L36 P TYPE LOWER PLANE P37 P TYPE UPPER 3363.33 5766.67 -500.00 TEST POINT END DEF #SFZ10b BEGIN\_DEF ZONE NAME Z37 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U37 P TYPE UPPER PLANE L37 P\_TYPE LOWER PLANE P36 P TYPE UPPER

TEST POINT 4603.33 11340.00 -500.00 END DEF #SFZ11 BEGIN DEF ZONE NAME Z38 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U38 P TYPE UPPER PLANE L38 P TYPE LOWER PLANE P5 P TYPE UPPER PLANE P2 P TYPE UPPER 5926.67 6496.67 -500.00 TEST\_POINT END DEF #SFZ13a BEGIN DEF ZONE NAME Z39 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U39 P TYPE UPPER PLANE L39 P TYPE LOWER PLANE P31 P TYPE UPPER PLANE P40 P TYPE LOWER TEST POINT 803.33 8713.33 -500.00 END\_DEF #SFZ13b BEGIN DEF ZONE NAME Z40 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U40 P TYPE UPPER PLANE L40 P TYPE LOWER PLANE P39 P TYPE LOWER PLANE P23 P TYPE LOWER TEST POINT 2196.67 8220.00 -500.00 END DEF #SFZ14a BEGIN DEF ZONE NAME Z41 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U41 P TYPE UPPER PLANE L41 P TYPE LOWER PLANE P35 P TYPE LOWER PLANE P42 P TYPE UPPER TEST POINT 1031.67 7415.00 -500.00 END DEF #SFZ14b BEGIN DEF ZONE NAME Z42 ALFA -7.41 BETA 0.0 STORATIVITY 1.0 PLANE U42 P TYPE UPPER PLANE L42

P TYPE LOWER PLANE P41 P TYPE UPPER PLANE P39 P\_TYPE UPPER TEST POINT 1185.00 8286.67 -500.00 END DEF #SFZ15 BEGIN DEF ZONE NAME Z43 ALFA -5.88 BETA 0.0 STORATIVITY 1.0 PLANE U43 P TYPE UPPER PLANE L43 P TYPE LOWER PLANE P32 P TYPE LOWER TEST POINT 2635.00 12103.33 -500.00 END\_DEF #EW-5 SRD5 BEGIN\_DEF ZONE NAME Z46 ALFA -7.61 BETA 0.0 STORATIVITY 1.0 PLANE Q1 P TYPE UPPER PLANE Q2 P TYPE LOWER PLANE Q3 P TYPE LOWER PLANE Q4 P\_TYPE UPPER PLANE Q5 P TYPE UPPER PLANE Q6 P TYPE LOWER TEST POINT 2190.00 7315.00 -350.00 END DEF #Fix SRD-zoner BEGIN DEF PLANE NAME F04 0.00000 0.00000 1.00000 EQUATION 600.000 TYPE UPPER END\_DEF #SRD1 BEGIN DEF ZONE NAME Z57 ALFA -8.03 BETA 0.0 STORATIVITY 1.0 PLANE P23 P TYPE UPPER PLANE P1 P TYPE LOWER PLANE P41 P\_TYPE UPPER PLANE P42 P TYPE UPPER PLANE F04 P TYPE LOWER TEST POINT 1600.00 7700.00 -300.00 END DEF #SRD1 BEGIN DEF ZONE NAME Z58 ALFA -9.03 BETA 0.0 STORATIVITY 1.0 PLANE P23 P TYPE UPPER PLANE P1

P TYPE LOWER PLANE P41 P TYPE UPPER PLANE P42 P TYPE UPPER PLANE F04 P TYPE UPPER TEST POINT 1600.00 7700.00 -1000.00 END DEF #SRD2 BEGIN DEF ZONE NAME Z59 ALFA -7.11 BETA 0.0 STORATIVITY 1.0 PLANE P1 P TYPE UPPER PLANE P23 P TYPE UPPER PLANE P2 P\_TYPE LOWER PLANE P41 P TYPE UPPER PLANE F04 P TYPE LOWER TEST POINT 1700.00 7400.00 -100.0 END DEF #SRD2 BEGIN DEF ZONE NAME Z60 ALFA -8.11 BETA 0.0 STORATIVITY 1.0 PLANE P1 P\_TYPE UPPER PLANE P23 P TYPE UPPER PLANE P2 P TYPE LOWER PLANE P41 P TYPE UPPER PLANE F04 P TYPE UPPER #TEST POINT 1900.00 7300.00 -1000.0 END DEF #SRD3 BEGIN DEF ZONE NAME Z61 ALFA -8.76 BETA 0.0 STORATIVITY 1.0 PLANE P2 P TYPE UPPER PLANE P5 P TYPE LOWER PLANE P24 P\_TYPE UPPER PLANE P3 P TYPE LOWER PLANE F04 P TYPE LOWER #TEST\_POINT 2400.00 7400.00 -500.0 END DEF #SRD3 BEGIN DEF ZONE NAME Z62 ALFA -9.76 BETA 0.0 STORATIVITY 1.0 PLANE P2 P TYPE UPPER PLANE P5 P TYPE LOWER PLANE P24 P TYPE UPPER

PLANE P3 P TYPE LOWER PLANE F04 P TYPE UPPER #TEST\_POINT 2400.00 7400.00 -700.0 END DEF #SRD4 BEGIN DEF ZONE NAME Z63 ALFA -7.54 BETA 0.0 STORATIVITY 1.0 PLANE P41 P TYPE UPPER PLANE P3 P TYPE UPPER PLANE P38 P TYPE UPPER PLANE P8 P TYPE LOWER PLANE P36 P\_TYPE LOWER PLANE F04 P TYPE LOWER #TEST\_POINT 2000.00 6500.00 -500.0 END DEF #SRD4 BEGIN DEF ZONE NAME Z64 ALFA -8.54 BETA 0.0 STORATIVITY 1.0 PLANE P41 P\_TYPE UPPER PLANE P3 P TYPE UPPER PLANE P38 P TYPE UPPER PLANE P8 P TYPE LOWER PLANE P36 P TYPE LOWER PLANE F04 P\_TYPE UPPER #TEST\_POINT 2000.00 6500.00 -700.0 END DEF #SRD4 BEGIN\_DEF ZONE NAME Z65 ALFA -7.54 BETA 0.0 STORATIVITY 1.0 PLANE P5 P TYPE UPPER PLANE P3 P TYPE LOWER PLANE P38 P\_TYPE UPPER PLANE F04 P TYPE LOWER #TEST POINT 2400.00 7150.00 -500.0 END DEF #SRD4 BEGIN DEF ZONE NAME Z66 ALFA -8.54 BETA 0.0 STORATIVITY 1.0 PLANE P5 P\_TYPE UPPER PLANE P3 P TYPE LOWER PLANE P38 P TYPE UPPER PLANE F04

**#**P\_TYPE UPPER TEST\_POINT 2400.00 7050.00 -700.0 END DEF #SRD4 BEGIN\_DEF ZONE NAME  $\overline{Z}67$ ALFA -7.54 BETA 0.0 STORATIVITY 1.0 PLANE P8 P\_TYPE UPPER PLANE P4 P\_TYPE LOWER PLANE P36 P TYPE LOWER PLANE P38 P\_TYPE UPPER PLANE F04 P\_TYPE LOWER #TEST\_POINT 3172.00 6709.00 -500.0 END\_DEF #SRD4 BEGIN DEF ZONE NAME Z68 ALFA -8.54 BETA 0.0 STORATIVITY 1.0 PLANE P8 P\_TYPE UPPER PLANE P4 P\_TYPE LOWER PLANE P36 P TYPE LOWER PLANE P38 P\_TYPE UPPER PLANE F04 P\_TYPE UPPER #TEST\_POINT 3244.00 6681.00 -700.0 END\_DEF END\_BLOCK

## Appendix H - Coordinate System Transformations

The simulations for Aberg are performed using coordinates in the Äspö local system. This means that all input data in form of e.g. stream tube starting positions and fracture zones are defined for that system. The model is set up in the Äspö local system with the origin for the model cube at (950, 6150, -1250). The HYDRASTAR modelling terms "user system" and "world system" are defined using that point in the Äspö local system. The HYDRASTAR "cube system" is not rotated in relation to the Äspö system. The used definitions of coordinate systems give output data for e.g. exit locations, which could be extracted from the lines\_<real>.hyp files, in the Äspö local system.

The Äspö local coordinate system is rotated 11.655 degrees west according to Walker et al. (1997) with an off-set of 1,550,827 and 6,360,252 in east and north, in relation to RAK. The coordinate systems for Aberg are right-handed with X toward east and Y toward north. The Z-direction is given in meter above sea level (m.a.s.l). To transform the modelling coordinates to RAK, the following equations have been used:

 $X_{RAK} = X_{Off-set} + X_A * \cos\theta - Y_A * \sin\theta$ 

 $Y_{RAK} = Y_{Off\text{-set}} + X_A * \sin\theta + Y_A * \cos\theta$ 

where  $X_{RAK}$  and  $Y_{RAK}$  stand for east and north, respectively,  $X_A$  and  $Y_A$  are Aberg modelling coordinates,  $X_{Off-set} = 1,550,827$ ,  $Y_{Off-set} = 6,360,252$  and,  $\theta = 11.655$  degrees.

A slightly different transformation is used for the repository layout prescribed by Munier et al. (1997). Adapting their transformation into the preceding form, the Munier et al. (1997) transform is:

 $X_{RAK38} = 1,551,210.173 + 0.978799*(X_A-1956.68) - 0.204822*(Y_A-7484.309)$ 

 $Y_{RAK38} = 6,367,978.295 + 0.204822*(X_A-1956.68) + 0.978799*(Y_A-7484.309)$ 

That is, Munier et al. (1997) use a rotation angle  $\theta$  of 11.819 degrees and an off-set of 1,551,210 and 6,367,978 in east and north, respectively. Munier et al. (1997) also use a local off-set of 1957 and 7484 in the local Äspö system. The differences between the Munier et al. (1997) system and the system used in this study is less than 25m (in terms of RAK-system coordinates) when calculating exit location using both set of equations.

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- <sup>2</sup> Bergab Consulting Geologists
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