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Hydrogeological boundary settings in SR 97

Uncertainties in regional boundary settings and transfer of boundary conditions to site-scale models

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Golder Grundtenik

June 1999

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Keywords: SR 97, Groundwater Modelling, Boundary Conditions, Uncertainty.

ABSTRACT

The SR 97 project presents a performance assessment (PA) of the overall safety of a hypothetical deep repository at three sites in Sweden arbitrarily named Aberg, Beberg and Ceberg. One component of this PA assesses the uncertainties in the hydrogeological modelling. This study focuses on uncertainties in boundary settings (size of model domain and boundary conditions) in the regional and site-scale hydrogeological modelling of the three sites used to simulating the possible transport of radionuclides from the emplacement waste packages through the host rock to the accessible environment. Model uncertainties associated with, for instance, parameter heterogeneity and structural interpretations are addressed in other studies. This study concludes that the regional modelling of the SR 97 project addresses uncertainties in the choice of boundary conditions and size of model domain differently at each site, although the overall handling is acceptable and in accordance with common modelling practice. For example, the treatment of uncertainties with regard to the ongoing post-glacial flushing of the Baltic Shield is creditably addressed although not exhaustive from a modelling point of view. A significant contribution of the performed modelling is the study of nested numerical models, i.e., the numerical interplay between regional and site-scale numerical models. In the site-scale modelling great efforts are made to address problems associated with (*i*) the telescopic mesh refinement (TMR) technique with regard to the stochastic continuum approach, and (*ii*) the transfer of boundary conditions between variable-density flow systems and flow systems that are constrained to treat uniform-density flow. This study concludes that the efforts made to handle these problems are acceptable with regards to the objectives of the SR 97 project.

SAMMANFATTNING

SR 97 utgör en av flera redovisningar av den långsiktiga säkerheten för inkapslat bränsle och annat långlivat avfall, deponerat i djupförvar. Syftet med SR 97 är att visa säkerhetsfunktionen för de geologiska förhållanden som kan förkomma inom tre möjliga förläggningsplatser, i svensk kristallin berggrund, och för den förvarsutformning som anpassats till dessa platser. De tre områdena som studeras i SR 97 kallas för Aberg, Beberg och Ceberg, vilka baserar sig på data från tidigare platsundersökningar utförda på uppdrag av Svensk Kärnbränslehantering AB (SKB). En komponent inom SR 97 är redovisningen av förekommande osäkerheter i samband med hydrogeologisk modellering och simulering av transport av radionuklider från inkapslat bränsle via grundvattenrörelser till biosfären. Denna studie är en sammanställning av olika osäkerheter ifråga om val av modelldomäner och randvillkor i samband med regional och platsspecifik modellering av de tre områdena. Hydrogeologiska osäkerheter som kan knytas till parameterheterogenitet och strukturgeologiska egenskaper behandlas inte i denna studie utan finns redovisade i andra rapporter.

I denna studie görs bedömningen att hanteringen av osäkerheter vid val av randvillkor och storlek på modellområde skiljer sig mellan de tre platserna, men att arbetssättet är tillfyllest för SR 97 och följer vedertagen praxis inom kunskapsområdet. Som exempel kan nämnas att hanteringen av osäkerheter i samband med den postglaciala landhöjningen med tillhörande ursköljning av salt grundvatten bedöms som trovärdig om än inte uttömmande ur modelleringssynpunkt. Ett väsentligt bidrag från SR 97 är hanteringen av osäkerheter som uppkommer vid överföringen av randvillkor mellan regional och platsspecifik numerisk modellering. I den platsspecifika modelleringen görs stora ansträngningar att hantera problem som uppstår i samband med (*i*) stokastisk kontinuummodellering i olika skalor och (*ii*) övergången från regionala system med variabel vattendensitet till platsspecifika system med konstant vattendensitet. I denna studie görs bedömningen att hanteringen av dessa problem är tillfyllest för SR 97.

EXECUTIVE SUMMARY

Uncertainties in hydrogeological boundary settings should be looked into by means of sensitivity studies. In practical work this implies simulations with alternative processes, boundary conditions and even different sizes of the model domain. Generally speaking, however, most sensitivity studies dealing with groundwater flow focus on parameter heterogeneity mainly. The hydrogeological modelling performed in the SR 97 project constitutes an exception in this respect. The SR 97 project contributes significantly to the study of nested numerical models, i.e., the numerical interplay between regional and site-scale numerical models. In particular, great efforts are made to address problems associated with (*i*) the telescopic mesh refinement (TMR) technique with regards to the stochastic continuum approach, and (*ii*) the transfer of boundary conditions between variable-density flow systems and flow systems that are constrained to treat uniform-density flow.

The three sites treated in SR 97, arbitrarily named Aberg, Beberg and Ceberg, are all situated below the highest marine shore level of the Baltic Sea. Ceberg is located in an area of Sweden, which has been and will be subjected to great shore level displacements. For example, during the next 10 000 years the total shore level displacement at Ceberg can be estimated to about 50 m, which is roughly a 50% increase of the present-day elevation. The corresponding values for Beberg and Aberg can be estimated to 40 m (~100%) and 15 m (~100%).

It is concluded that the post-glacial flushing of the Baltic Shield is an important transient hydrogeological process that may incorporate variable-density flow. The canister defect scenario (CDS) of the SR 97 project, however, postulates a simplification of the present-day situation for the site-scale hydrogeological modelling, i.e., steady state flow and a uniform-density fluid. The overall rationale for this simplification is discussed in other studies. This study discusses its hydrogeological relevance and implications.

Regarding the regional hydrogeological modelling performed for the SR 97 project it may be concluded that the historical hydrogeological evolution is modelled differently at the three sites, although the overall handling is acceptable and in accordance with common modelling practice. For instance, at Aberg steady state variable-density flow is simulated, whereas at Beberg transient variable-density flow is simulated, and at Ceberg steady state uniform-density flow is simulated. At Aberg uncertainties in the size of the regional hydrogeological domain (RHD) and the type of boundary conditions are not examined. On the other hand, the size of the regional model domain at Aberg is very large, which probably puts the target area of interest sufficiently far away from the regional boundaries. At Beberg, the size, of the RHD is not varied but the lateral boundary conditions are modelled as dynamic in order to simulate the effect of changing groundwater conditions due to the post-glacial shore level displacement and subsequent variable-density flow. At Ceberg, steady state uniform-density flow is assumed while studying two different sizes of the regional hydrogeological domain as well as a number of different types of top boundary conditions.

The importance of taking variable-density flow into account is well demonstrated in the regional hydrogeological modelling performed at Aberg and Beberg. Both studies show that saline conditions may affect the location of discharge areas as well as the travel time calculations. At Beberg, the concentrations and the pressures on the lateral sides are modelled as transient and the top boundary is modelled as specified pressure and zero concentration. At Aberg, the lateral boundaries are modelled as constant pressure and concentration in time. Here the top boundary is modelled as constant flux and zero concentration in the terrestrial parts, and as constant pressure and concentration in the marine parts.

The regional modelling performed at Ceberg addresses the size problem, i.e., two different sizes of the regional hydrogeological domain (RHD) are examined. The results suggest that the smaller domain captures the body of the discharge areas found in the larger domain simulation. It may be noted that at Beberg, which is comparable in size but modelled quite differently due to the presence of saline groundwater, the chosen RHD is shown to be too small in order to capture all of the discharge.

The justification for assuming steady state flow of a uniform-density fluid at Ceberg is based on the finding that a majority of SKB's measurements in deep boreholes at Ceberg indicate fresh groundwater conditions.

As mentioned previously, the CDS postulates a simplified present-day situation for the site-scale hydrogeological modelling. It should be noted that it might not be possible to estimate the total uncertainty imbedded in this conjecture without more modelling. For the sake of future studies on this matter, the following modelling procedure may be suggested as a means of addressing the uncertainty of the CDS more firmly:

1. The post-glacial flushing of the Baltic Shield is modelled at each site using transient boundary conditions and variable-density flow. However, unlike the modelling performed at Beberg the simulations should not be halted at the present-day situation but continued until the specified time limit of the performance assessment period is reached.
2. The simulated conditions, at various times, are visualised and compared with the simulated present-day conditions.

The proposed modelling procedure will allow for more detailed judgements regarding spatial and temporal differences in the discharge, which may be different from (or comparable to) those of a present-day assumption.

The conclusions above relate to the performance of the regional hydrogeological modelling mainly. Uncertainties in the interplay between regional and site-scale hydrogeological modelling are also treated in the SR 97 project. Two main types of uncertainty are handled in the site-scale modelling. The first one concerns parameter uncertainty with regards to the application of the telescopic mesh refinement (TMR) technique in flow systems that are modelled with the stochastic continuum approach. The second one belongs to the transfer of boundary conditions between variable-density flow systems and flow systems that are constrained to treat uniform-density flow.

The simulations of variable-density flow on the regional scale are based on pressure as a state variable, whereas the site-scale simulations in CFS are based on hydraulic heads and uniform-density flow. Before the conversion from pressures to heads is made it is important to conclude whether the gradient of flow in the regional simulations is mainly vertical or horizontal. If the salinity gradient is mainly vertical (stratified salinity) one may consider using environmental heads rather than fresh-water heads. However, if the horizontal gradient is more important one may use fresh-water heads instead. If fresh-water heads are used in a situation where the salinity field is stratified then the vertical hydraulic gradients may be exaggerated. This study concludes that the efforts made to handle this problem is acceptable with regards to the objectives of the SR 97 project.

CONTENTS

1 GENERAL

1.1 Introduction

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 in crystalline rock. The SR 97 project presents a performance assessment (PA) of the overall safety of a deep repository at three hypothetical sites in Sweden arbitrarily named Aberg, Beberg and Ceberg. One component of this PA assesses the uncertainties in the hydrolgeological modelling used to simulating the possible transport of radionuclides from the emplacement waste packages through the host rock to the accessible environment (Andersson et al., 1996).

1.2 Objectives and Scope of Work

A key hydrogeological parameter in PA is groundwater flux (volumetric flow rate per unit area). Groundwater flux is important for both near-field (source strength) and far-field (advective travel time) calculations. According to Darcy's law, the product of the hydraulic conductivity of the medium and the hydraulic gradient determines the flux through a geologic medium across the inflow and outflow faces in the direction of flow. In numerical modelling of groundwater flow the boundary settings (size of model domain and boundary conditions) determine the location of the recharge and discharge areas in large as well as the direction and magnitude of the global hydraulic gradient.

This study examines the choice of boundary settings used in the regional hydrogeological modelling of Aberg, Beberg and Ceberg. Hydrogeological uncertainties associated with, for instance, parameter heterogeneity and structural interpretations are addressed in other studies. Moreover, the study examines the conceptual and numerical interplay between regional and site-scale groundwater modelling. The approach used by SKB in the SR 97 project is in the literature called the telescopic mesh refinement (TMR) technique.

1.3 Previous Work

The regional groundwater modelling of Aberg, Beberg and Ceberg is made by Svensson (1997), Hartley et al. (1998) and Boghammar et al. (1997). These three studies constitute the main sources of information for the regional scale issues of the present study. Other regional studies of interest are the structural-geological review by Saksa and Nummela (1998) and the hydrogeological data report by Walker et al. (1997).

The site-scale modelling of Aberg, Beberg and Ceberg is made by Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999). These three studies constitute the main sources of information for the site-scale issues of the present study. Another study of interest is the report on preparatory calculations for the site-scale models by Gylling et al. (1999b).

1.4 Layout of Report

After the introduction in Chapter 1 the report follows, essentially, the proposed layout of Hedin (1997a,b). Chapter 2 presents an overview of various types of boundary conditions and the rationale for their use in numerical modelling of groundwater flow. The overview may serve as a guidance or reference for the inexperienced reader. Chapter 2 also discusses the interplay between boundary conditions and other parameters and how uncertainties may be dealt with. Chapter 3 presents the SR 97 modelling approach. Chapter 4 presents the choice of regional hydrogeological domain and boundary conditions in the performed regional hydrogeological modelling of Aberg, Beberg and Ceberg. Chapter 4 also discusses certain and possible uncertainties in the performed regional modelling. Chapter 5 discusses uncertainties in the interplay between regional and site-scale models, in particular, uncertainties associated with the telescopic mesh refinement (TMR) technique, transfer of boundary conditions to the site-scale model, and variable-density flow.

2 BOUNDARY SETTINGS - DEFINITIONS AND INTERPLAY WITH MODEL PARAMETERS

2.1 General

Mathematical models consist of a governing equation, boundary conditions, and initial conditions. In hydrogeological modelling of groundwater flow, boundary conditions are mathematical statements specifying the dependent variable (pressure; hydraulic head) or the derivative of the dependent variable (flux) at the boundaries of the problem domain. Some typical boundaries for two- and three-dimensional problem domains are shown in Figure 2-1.

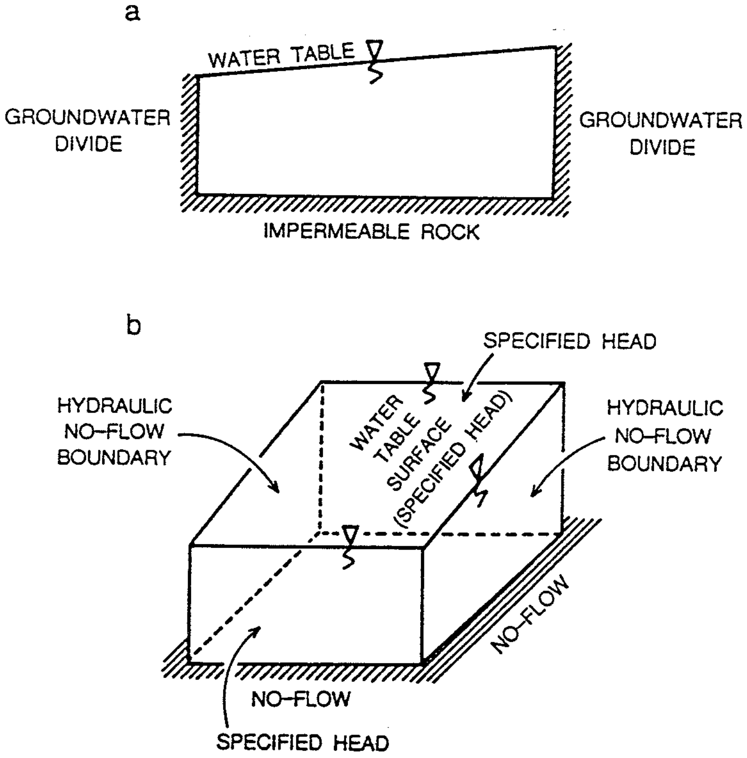


Figure 2-1 Typical boundaries in regional flow problems.
(a) Two-dimensional problem in profile view.
(b) Three-dimensional problem domain.
(Anderson and Woessner, 1992.)

In steady state flow simulations, the boundary conditions largely determine the flow pattern and the location of recharge and discharge areas. Boundary conditions influence transient solutions when the effects of the transient stress reaches the boundary, which means that the boundaries must be selected so that the simulated effect is realistic.

Franke and Reilly (1987) studied the effect of boundary conditions on the steady state response of three hypothetical ground-water systems. These results and others indicate that —

1. Different boundary conditions define different groundwater systems, even if the geometry and hydraulic conductivity of the systems are identical. In other words, if a simulated groundwater system has incorrect boundary conditions (conditions that do not correspond to those in the natural system under study), then the simulation exercise is solving the wrong problem and, by definition, will provide the wrong solution.

2. Model calibration with respect to heads alone is not reliable for unstressed steady state analyses but tends to improve in stressed systems. In stressed and unstressed systems, however, correct boundary conditions are essential to the representation of sources of water and patterns of flow within the system. Thus, incorporating measurements and estimates of groundwater flow from the natural system in the process of model development and assessment of its acceptability (the calibration process) is of utmost importance.

3. The effect of boundary conditions on system response should be considered at every phase of an investigation involving simulation, including the calibration phase, which should include sensitivity analyses on arbitrarily selected boundary conditions.

Franke and Reilly (1987) advocate that setting boundary conditions is the step in model design that is most subject to serious error. Uncertainties in the boundary settings should be looked into by means of sensitivity studies. In practical work this implies simulations with different boundary conditions and even different sizes of the model domain.

2.2 Types of Boundaries

For the purpose of this report, we make a short review of the terminology and rationale concerning hydrogeological boundary conditions and modelling.

Physical boundaries of groundwater flow systems are formed by the physical presence of an impermeable body of rock or a large body of surface water. Other boundaries form as a result of hydrologic conditions. These invisible boundaries are hydraulic boundaries that include groundwater divides and streamlines.

For example, in Figure 2-2 two regional flow systems are bounded by physical boundaries: impermeable rock at the bottom, the water table at the top, and the rivers along part of the side boundaries (ABC in the inset). Groundwater divides form hydraulic boundaries whose locations are influenced by the presence of physical features – topographic lows that hold major rivers and a topographic high. On the left-hand side of the diagram, shallow local flow systems are separated from an intermediate flow system by dividing streamlines that form no-flow hydraulic boundaries. The intermediate flow system is separated from the regional flow system by another dividing streamline. All hydraulic boundaries, including those that coincide with physical features, are transitory features that may shift location or disappear altogether if hydrologic conditions change.

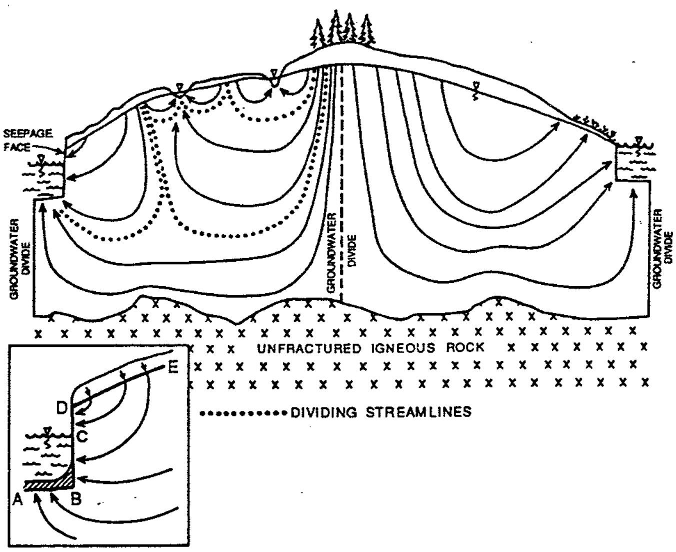


Figure 2-2 Regional flow systems showing physical and hydraulic boundaries. The inset shows a close-up of several types of boundaries. The river boundary (ABC) could be treated as a specified head boundary, a specified flow boundary, or a head-dependent flow boundary. The seepage face forms a boundary along CD and the water table forms the boundary along DE. Bedrock forms a physical boundary to groundwater flow. (Anderson and Woessner, 1992.)

Hydrogeological boundaries are represented by the following three types of mathematical conditions:

1. *Specified head boundaries* for which head is given.

2. *Specified flow boundaries* for which the derivative of head (flux) across the boundary is given. A no-flow boundary condition is set by specifying flux to be zero.

3. *Head-dependent flow boundaries* for which flux across the boundary is calculated given a boundary head value. This type of boundary condition is sometimes called mixed boundary condition because it relates boundary heads to boundary flows. There are several types of head-dependent flow boundaries.

2.3 Some Aspects on Setting Boundaries

When selecting boundaries the modeller should visualise the probable flow pattern that will be induced by the boundaries and determine whether the flow pattern makes sense. For instance, does the inflow and outflow locations agree with the general recharge and discharge areas observed in the field? It is advisable to select physical boundaries whenever possible because they usually are stable features of the flow system.

Impermeable rock typically forms boundaries of a modelled system. A two order of magnitude contrast in hydraulic conductivity may be sufficient to justify placement of an impermeable boundary. This type of contrast in hydraulic conductivity causes refraction of flow lines such that flow occurs mainly in the higher-conductivity rock. If hydraulic gradients across the boundary are also low, flow out of the higher-conductivity rock will be negligible, and the boundary can be considered impermeable. If leakage across the boundary is significant, boundary fluxes or heads can be specified, if known. Otherwise, it will be necessary to incorporate (simulate) the lower-conductivity rock and expand the modelling domain until a better defined boundary can be identified. Surface water bodies form ideal specified head boundaries. Termination of model to an impermeable fault zone forms a convenient physical no-flow boundary.

It may not be possible or convenient to design a grid that includes the physical boundaries of the system if the focus of interest is far removed from the boundaries. In this case, it may be possible to identify a regional groundwater divide closer to the area of interest, which could be used as a no-flow boundary. Regional groundwater divides are typically found near topographic highs and may form beneath partially penetrating surface water bodies (Figure 2-2). Although hydraulic boundaries are not stable features of the flow system, regional groundwater divides are likely to be more permanent than other types of hydraulic boundaries.

A flow system will usually have a mix of specified head and specified flow boundaries but occasionally the conceptual model of the problem may be formulated entirely with flux boundaries. Although hydrogeological defensible, exclusive use of flux boundaries generally should be avoided for the following mathematical reason. The governing equation is written in terms of derivatives, or differences in head, so the solution will be non-unique if the boundary conditions also are specified as derivatives. Steady state problems require at least one boundary node with a specified head in order to give the model a reference elevation from which to calculate heads. In transient solutions, the initial conditions provide the reference elevation for the head solution so that the use of all flux boundaries may be justified for certain types of problems.

If it is not possible to use physical boundaries and regional groundwater divides, it will be necessary to select other boundaries. These are typically hydraulic boundaries defined from information on the configuration of the flow system. Care must be taken when defining such boundaries to demonstrate both conceptually and numerically that the model boundaries will not cause the solution to differ significantly from the response that would occur if physical boundaries and regional groundwater divides were used. When documenting model results, the physical boundaries of the regional flow system should be identified as precisely as possible even if they are distant from the area of concern and are not included in the model.

Hydraulic boundaries that do not coincide with regional boundaries or do not relate to information on the configuration of the flow system are sometimes called artificial boundaries. Such boundaries are frequently used to create a smaller problem domain. Artificial boundaries can be set using a modelling procedure termed telescopic mesh refinement (TMR). Using telescopic mesh refinement, a grid with coarse nodal spacing is fitted to the regional boundaries, and boundary conditions for a refined model covering a smaller geographic area (site-scale domain) are defined from the regional scale simulation. The TMR technique is envisaged in Figure 2-3.

The TMR technique implicitly assumes that the groundwater flow through the smaller model domain is unchanged. In practical words this means that if head values from the regional scale simulation are used as artificial boundaries on a smaller model domain, then the equivalent conductivity of the smaller model domain must equal that of the corresponding portion of the regional model domain.

Artificial boundaries can be used legitimately to produce a steady state flow field for calibration purposes. However, they may not be acceptable for steady state predictive simulations. This is because the model assumes that conditions on the boundaries do not change from their initial values unless the modeller during the simulation explicitly changes them.

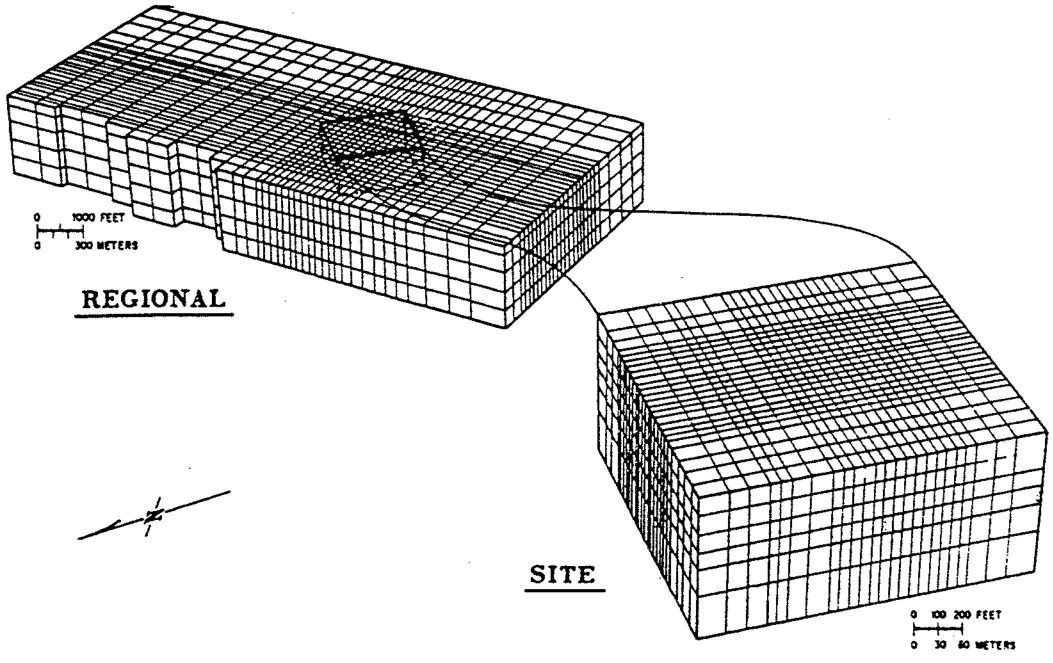


Figure 2-3 Illustration of the telescopic mesh refinement technique. (After Ward et al., 1987).

3 USE IN THE SR 97 PROJECT

3.1 Limitations and Uncertainties of the Canister Defect Scenario

The site-scale groundwater modelling part of the SR 97 project is restricted to handle the canister defect scenario (CDS). The hydrogeological form of this scenario is given by Hedin (1997a,b) and may be summarised as follows—

Present hydrological and geological conditions are assumed to prevail for a long period of time. Implications of this simplification should be discussed if the shore level displacement has a significant impact on the imposed boundary conditions.

Shore level displacement has been, and still is at some locations in Sweden, a process of major importance to the hydrology of the Baltic Shield (Voss and Andersson, 1993). Figure 3-1 gives an apprehension of the changes in the elevation in the past and in the future. The graph is based on a model provided by Påsse (1997) and shows the shore level displacement for Beberg. Figure 3-1 suggests a continuous displacement of the recharge and discharge conditions, although the rate of the displacement is decreasing with time. Figure 3-1 also suggests that the present-day groundwater conditions may not be at steady state. Shore level displacement may be more important for the regional hydrogeological modelling of Ceberg and Beberg than for Aberg if forthcoming changes in ground elevation are considered only. However, in order to understand the present-day situation the historic evolution is probably equally important for all three sites (Voss and Andersson, 1993). According to the model by Påsse (1997) the total shore level displacement at Ceberg can be estimated to about 50 m during the next 10 000 years, which is approximately a 50% increase of the present-day elevation. The corresponding values at Beberg and Aberg can be estimated to 40 m (~100%) and 15 m (~100%).

The simplification of a homogeneous fluid may not always be true in Baltic Shield rock, at least not for sites that are situated below the highest marine shore level. The three sites dealt with in the SR 97 project are all situated below the highest marine shore level of the Baltic Sea. Hence, it may be concluded that the post-glacial flushing of the Baltic Shield is probably the single most important hydrogeological process to consider in a study such as the present one.

In conclusion, the uncertainties imbedded in the simplifications made in the CDS may not be possible to estimate without more modelling. The major reason for this limitation is that the performed regional hydrogeological modelling is either made at steady state (Aberg and Ceberg) or treated as transient but stopped at the present-day situation (Beberg). Hence, future developments of the flow field (flux magnitudes and orientations) as well as the location of future discharge areas are unknown. It is important to note, however, that the uncertainty about the future lays solely in the simplification postulated by the CDS and not in the quantitative modelling as such.

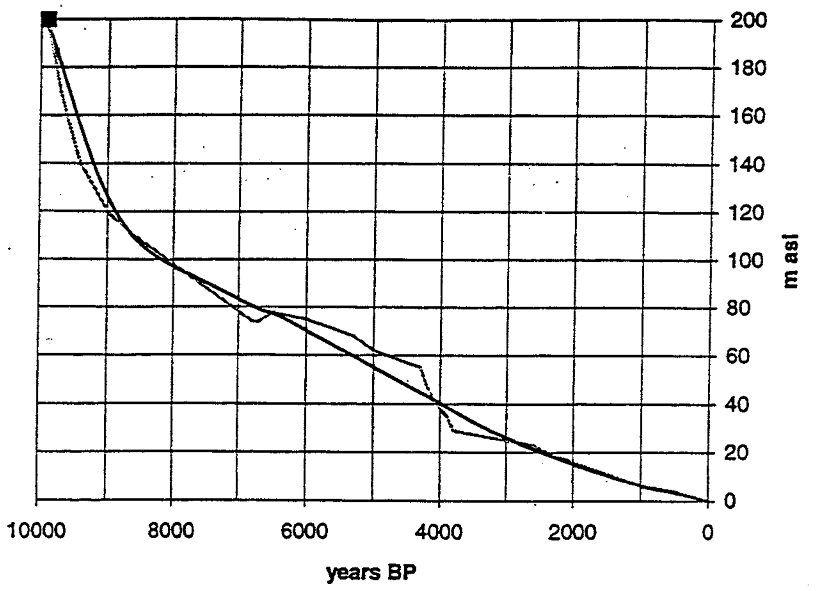
For the sake of future studies on this matter, the following modelling procedure may be suggested as a means of addressing the uncertainty of the CDS more firmly:

1. The post-glacial flushing of the Baltic Shield is modelled at each site using transient boundary conditions and variable-density flow. However, unlike the modelling performed at Beberg the simulations should not be halted at the present-day situation but continued until the specified time limit of the performance assessment period is reached.
2. The simulated conditions, at various times, are visualised and compared with the simulated present-day conditions.

3.2 SR 97 Modelling Approach

SKB uses a computer code called HYDRASTAR (Norman, 1992) for the derivation of hydrogeological input to the SR 97 PA calculations. HYDRASTAR is specifically developed by SKB for parameter heterogeneity simulations. However, HYDRASTAR cannot simulate a large model domain and simultaneously maintain a high resolution of the parameter heterogeneity. For this reason SKB has decided to use the TMR technique (cf. Figure 2-3). The TMR technique, as practised by SKB in the SR 97 project, may be summarised as follows—

1. For each of the three sites a regional domain is identified, which is much larger than the site domain where the deep repository is hosted.
2. The regional domains are turned into a regional numerical models using coarse nodal spacings (~ 100 m). The modeller determines the hydrogeological parameters and the boundary conditions for the chosen regional model domains. The finite-difference code PHOENICS (Spalding, 1981) is used for the regional modelling of Aberg (Svensson, 1997), whereas the finite-element code NAMMU (Cliffe et al., 1995) is used for the regional modelling of Beberg (Hartley et al., 1998) and Ceberg (Boghammar et al., 1997).
3. The regional models are explored in various ways. The cases studied in the SR 97 project are discussed in Chapter 4.
4. Hydraulic (and/or environmental) heads from the regional models are then used as boundary conditions for the corresponding site-scale model domains. The site-scale models use a much finer nodal spacing (~ 25 m) than the regional models (~ 100 m). Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) make the site-scale groundwater modelling of Aberg, Beberg and Ceberg. All site-scale modelling is made with the finite-difference code HYDRASTAR.
5. In the final step, each site-scale model is explored using the Monte Carlo method. In all the realisations, the boundary settings are kept constant while the conductivity field is varied from one realisation to the next in a random fashion by means of geostatistical correlations. Each site is studied with a Base Case and 1-4 variant simulations.



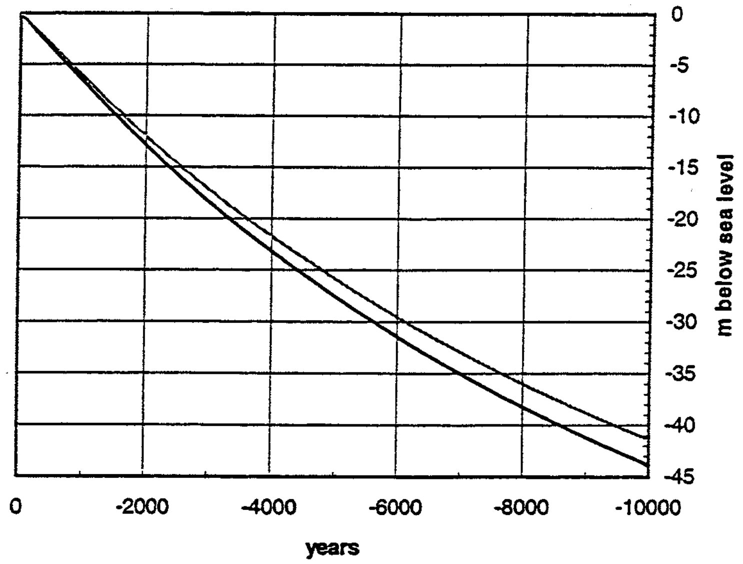


Figure 3-1 Shore displacements versus time for regions close to Beberg (After Påsse, 1997). The uppermost plot shows the calculated past displacement (solid line) with regards to obsolete pollen analytical datings (dotted line). The lowermost plot shows the predicted displacement (dotted line) and predicted isostatic rise (solid line).

3.3 Methodological uncertainties

The adaptation of the TMR technique to the SR 97 project described in Section 3.2 is an extension of what is generally seen in the literature in terms of TMR modelling (cf. Chapter 2). Widén and Walker (1998) used the outlined approach at Aberg in another study (AMP) for the SR 97 project. The authors found that the TMR technique may render individual realisations of the site-scale groundwater flow that differ slightly in flux (magnitudes and directions) compared to the result of the corresponding sub-domain in the regional model[1]. The authors found that the mean difference in groundwater flux was less than one order of magnitude for the conductivity heterogeneity observed at Aberg. This observation suggests that the uncertainty caused by the current adaptation of the TMR technique may be of moderate importance to the SR 97 project.

HYDRASTAR can handle the CDS but is limited in its ability to deal with other types of hydrogeological scenarios. Examples of difficult scenarios are irregular and mixed (Type 3) boundary settings, transient boundary conditions (shore level displacement), variable-density flow (salinity changes), hydraulic anisotropy (asymmetric fracturing) and a spatially varying porosity (uneven fracturing). The computer codes that SKB uses for the regional groundwater modelling are much more capable in this respect. Due to the physical importance of variable-density flow at Aberg and Beberg, there are uncertainties arising when the pressure solution of the regional domain is used as a hydraulic-head boundary condition in the site-scale hydrogeological modelling with HYDRASTAR. However, by using the concept of environmental head (Lusczynski, 1961) this problem is sufficiently handled in the site-scale hydrogeological modelling for the sake of the SR 97 project.

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[1] One reason for this discrepancy is that the boundary conditions used for the site-scale groundwater simulations (Step 4) become incorrect when changes are made to the hydraulic conductivity field (Step 5).

4 UNCERTAINTIES IN REGIONAL BOUNDARY SETTINGS

4.1 General

This chapter focuses on uncertainties regarding the hydrogeological processes and boundary settings considered in the regional modelling of Aberg, Beberg and Ceberg.

Figures 4-1 through 4-3 show the geographical settings of Aberg, Beberg and Ceberg as well as the locations and sizes of the regional and site-scale model domains.

Table 4-1 presents a compilation of technical and hydrogeological settings used for numerical simulation of regional groundwater flow. The information in this table is a condensation of the documentation of the regional groundwater modelling of Aberg, Beberg and Ceberg by Svensson (1997), Hartley et al. (1998) and Boghammar et al. (1997).

Table 4-1 shows that the regional modelling in terms of boundary conditions and size of model domain is treated differently at each site. However, the overall handling of the identified uncertainties in the boundary settings is in accordance with common modelling practice. For example, the treatment of uncertainties with regard to the ongoing post-glacial flushing of the Baltic Shield is creditably addressed for the sake of the SR 97 project although not exhaustive from a modelling point of view.

In the subsequent sections some points of interest to the present study are highlighted.

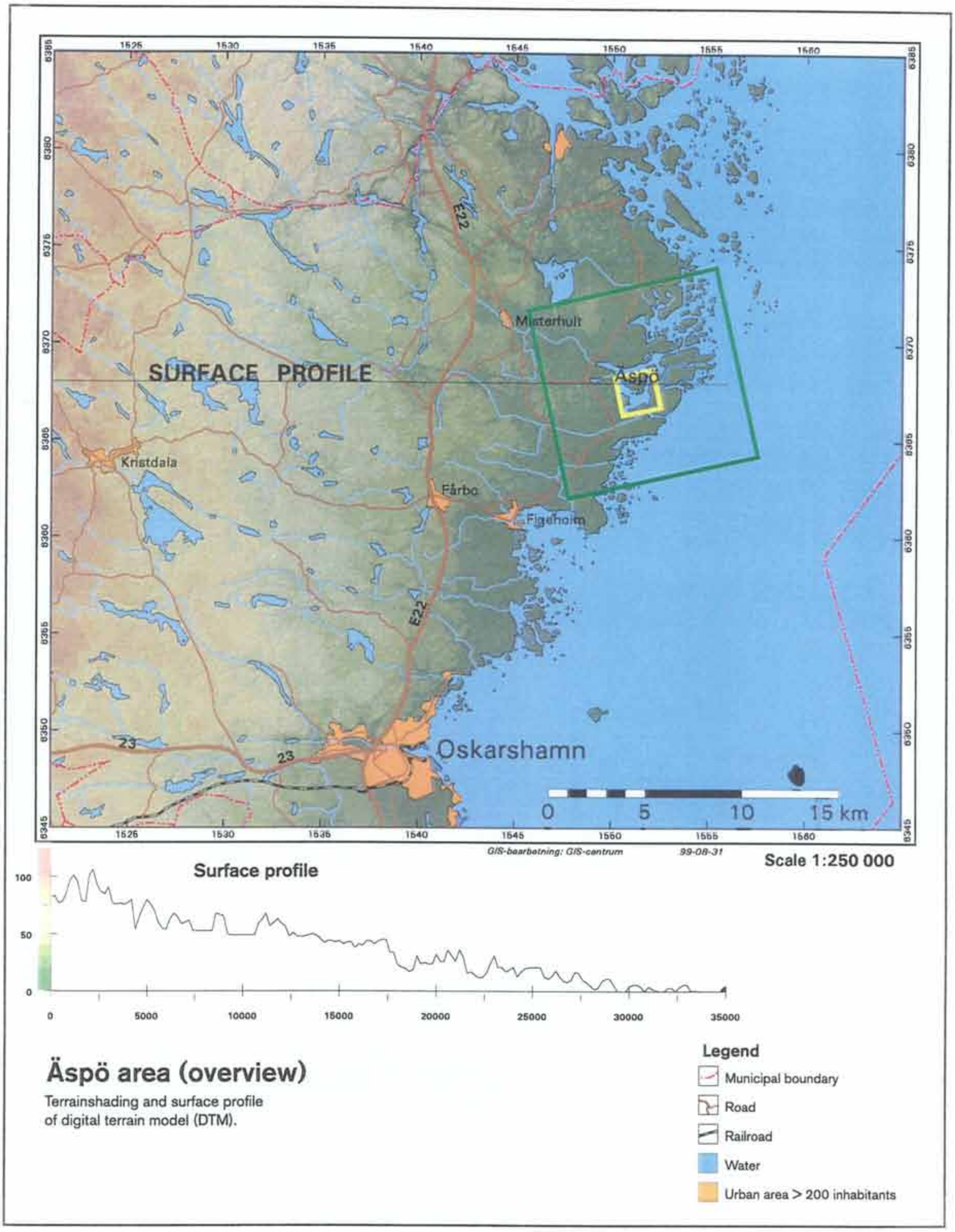

Figure 4-1 Geographical setting of Aberg. The rectangles show the location and size of the regional and site-scale hydrogeological model domains.

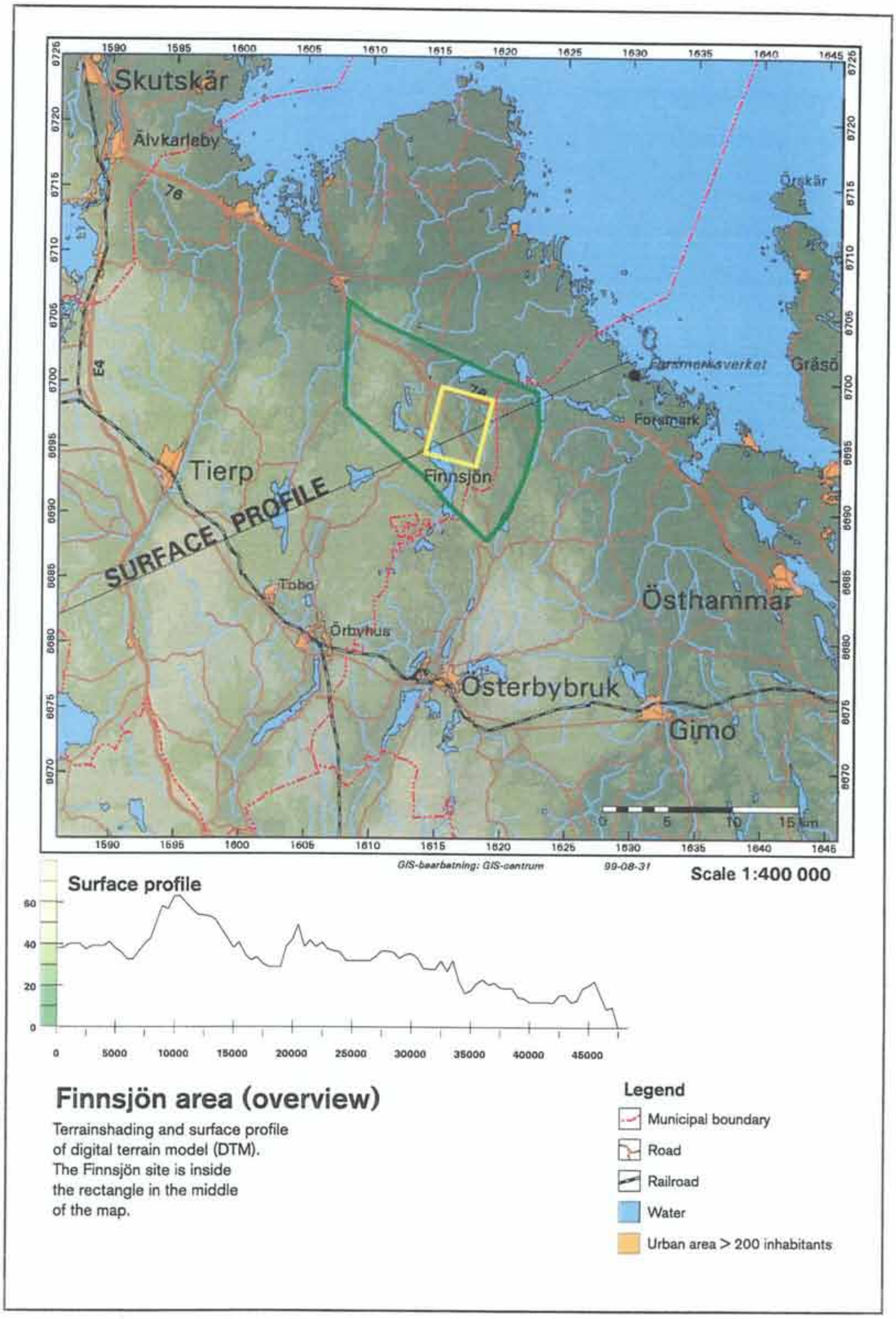

Figure 4-2 Geographical setting of Beberg. The rectangles show the location and size of the regional and site-scale hydrogeological modelling domains.

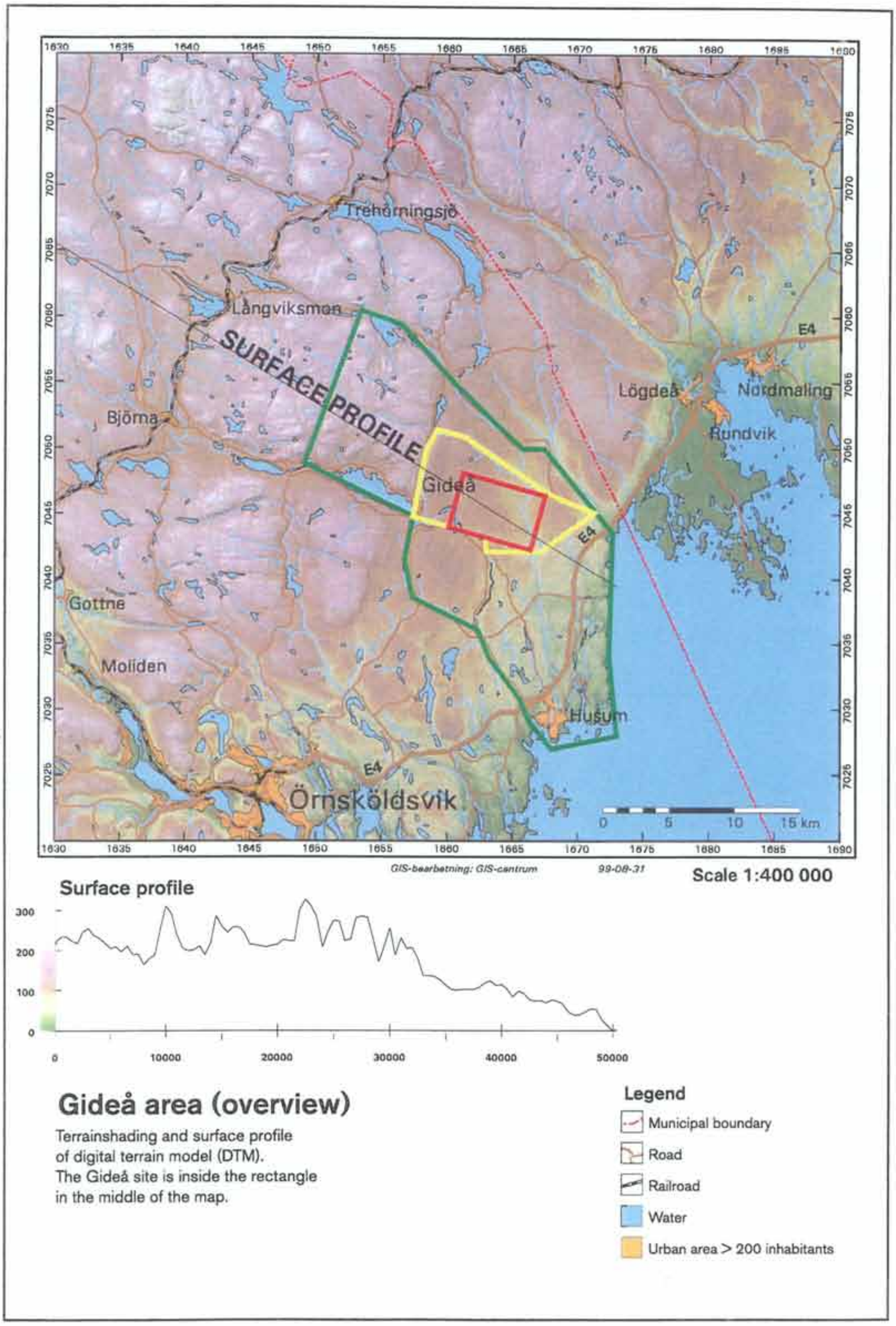

Figure 4-3 Geographical setting of Ceberg. The rectangles show the location and size of the regional and site-scale hydrogeological modelling domains. The regional modelling is performed for two different sizes of the model domain.

Table 4-1 Compilation of technical and hydrogeological settings for the numerical simulation of regional groundwater flow at Aberg, Beberg and Ceberg.

Object	***Aberg***	***Beberg***	***Ceberg***
Computer Code	PHOENICS	NAMMU	NAMMU
Type and size of the regional hydrogeological domain (RHD)	Fixed 10×10×3 km^3	Fixed 20×10×2 km^3	Varied 1. 30×10×1.5 km^3 2. 10×5×1.5 km^3
Is the location and size of the RHD based on structural boundaries	No	Yes	Yes
Type of simulation mode	Steady state	Transient	Steady state
Fluid condition	1. Variable-density flow	1. Variable-density flow 2. Shore level displacement	1. Uniform-density flow
Parameter Mode	Deterministic Single statistical realisation with parameter heterogeneity (K)	Deterministic Best estimate realisation with rock mass and explicit fracture zones	Deterministic Best estimate realisation with rock mass and implicit fracture zones
Bottom B.C.	Fixed No flow	Fixed No flow	Fixed No flow
Top B.C.	Fixed Specified infiltration. Zero concentration.	Fixed Specified head. Zero concentration.	Varied 1. Specified head 2. Specified infiltration 3. Head-dependent flux 4. Interpolated from larger regional model
Lateral B.C.	Fixed A combination of no flow and hydrostatic pressure. Fixed concentration.	Variable Transient hydrostatic pressure and concentration	Fixed A combination of No flow and hydrostatic head. Zero concentration

4.2 Aberg

Ideally, both the size of the regional hydrogeological domain (RHD) and the boundary conditions should be investigated in an uncertainty assessment study. At Aberg the size of the chosen RHD and the type of boundary conditions used are not discussed in detail. Moreover, the location of the RHD and the boundary conditions applied are not based on structural or hydraulic evidence (Saksa and Nummela, 1998). On the other hand, the size of the regional model domain at Aberg is very large, which probably puts the target area of interest sufficiently far away from the regional boundaries (cf. Voss and Andersson, 1993).

The regional hydrogeological situation at Aberg is modelled as variable-density flow at steady state. This implies that the post-glacial flushing of the rock is considered to be terminated and balanced by the present-day topography and salinity conditions in the Baltic Sea and below. According to Påsse (1997) the total shore level displacement at Aberg can be estimated to about 15 m during the next 10 000 years, which roughly means a 100% increase of the present-day elevation. This change in elevation exceeds the depth of the Baltic Sea around Aberg, which means the future distribution of recharge and discharge areas close to the shoreline will be different than the present-day distribution.

The hydrologic top boundary condition at Aberg is defined as specified infiltration over the terrestrial parts of the RHD in combination with the specified pressure over the marine parts. This setting implies no terrestrial discharge of deep groundwater at any location.

4.3 Beberg

At Beberg, the size of the RHD is held constant, but the location of the RHD is based on structural evidence. Moreover, the RHD coincides with the regional structural domain considered by Saksa and Nummela (1998). It may be noted that all major structures discussed by these authors are explicitly modelled as fracture zones. From a hydrogeological point of view, however, the location and size of the RHD may be discussed (cf. below).

The hydrogeological situation is modelled as variable-density flow with transient boundary conditions between 4 000 BP and today, which means that the post-glacial flushing of the rock during this period of time is treated as a continuous process. This is accomplished by altering the pressures on the lateral boundaries as the concentration of salt changes due to washout. Hartley et al. (1998) conclude, however, that the regional modelling of Beberg is too small in order to capture all of the discharge even for the present-day situation. This suggests that the simulated rate of the washout may be uncertain. Secondly, the top boundary is set to mimic the present-day groundwater table, which prohibits modelling of future changes in the shore level displacement. Although this modelling constraint is in accordance to the CDS it is interesting to note that during the next 10 000 years the total shore level displacement at Beberg can be estimated to about 40 m, which roughly means a 100% increase of the present-day elevation.

4.4 Ceberg

The regional hydrogeological modelling of Ceberg examines different sizes of the RHD. As for Beberg, the locations of the RHD are based on structural evidence, and the two RHD coincide with the body of the regional structural domain considered by Saksa and Nummela (1998). However, it may be noted that the hydraulic interpretations of the structures are not explicitly implemented as for Beberg. Instead, the modelled structures are implicitly taken into account by altering the rock mass conductivity.

The simulation results for Ceberg suggest that the smaller domain captures the body of the discharge areas found in the larger domain simulation. For the purpose of this study, it may be noted that the chosen RHD at Beberg, which is comparable in size but modelled quite differently, is shown to be too small in order to capture all of the discharge.

Although the body of SKB's measurements in deep boreholes at Ceberg indicates fresh groundwater conditions, the assumption of steady state, uniform-density flow may be highlighted. There are at least two borehole measurements that indicate saline groundwater conditions at depth. According to Ahlbom et al. (1991) saline groundwater has been observed in borehole KGI04 at 385 m (178 mg Cl^-/L), and 596 m (260 mg Cl^-/L). Ahlbom et al. (1991) conclude that the chemical compositions of these water samples indicate mixtures of recent surface waters and deep saline groundwater of unknown origin.

The salinity observations are moderate. Notwithstanding, they indicate that an alternative reconstruction of the hydrogeological conditions may take post-glacial flushing into account.

5 UNCERTAINTIES IN SITE-SCALE BOUNDARY SETTINGS

5.1 General

Two main types of uncertainties are handled in the SR 97 project regarding the interplay between regional and site-scale hydrogeological modelling. The first one concerns parameter uncertainty with regards to the application of the telescopic mesh refinement (TMR) technique in flow systems that are modelled with the stochastic continuum approach. The second one belongs to the transfer of boundary conditions between variable-density flow systems and flow systems that are limited to treat uniform-density flow.

The geographical settings of the site-scale model domains of Aberg, Beberg and Ceberg are shown in Figures 4-1 to 4-3. The site-scale hydrogeology of each site was modelled with a Base Case and a couple of variant simulations. The Base Case was based on expert opinion, which means that it represents the expected site conditions. Each of the variant simulations corresponds to a possible alternative interpretation of the site-scale hydrogeology.

This chapter focuses on uncertainties regarding the transfer of boundary conditions from the regional, variable-density flow models to the site-scale, uniform-density, Base Case variant models of Aberg, Beberg and Ceberg. Uncertainties regarding the size of the site-scale model domains are treated by Gylling et al. (1999b), whereas Walker and Gylling (1998), Gylling et al. (1999a) and Walker and Gylling (1999) handle parameter uncertainties with regards to the application of the telescopic mesh refinement (TMR) technique.

5.2 Hydraulic Head and Environmental Head

Due to the considerations made to variable-density flow for two of the regional studies (Aberg and Beberg) there are physical uncertainties arising when the pressure fields of the regional simulations are transferred to hydraulic head boundary conditions in the site-scale hydrogeological modelling. Lusczynski (1961) concludes that if the salinity gradient is mainly vertical (stratified salinity) one may consider using environmental heads (H_e) rather than freshwater heads (H_f) since the vertical flux (q_z) may be expressed as

$$q_z \propto \rho_f \left(\frac{\partial H_e}{\partial z} \right)$$

where ρ_f is the ambient fresh-water density. However, if the horizontal gradient is the most pronounced one may use fresh-water heads instead since the horizontal fluxes (q_x and q_y) may be expressed as

$$q_x \propto \rho_f \left(\frac{\partial H_f}{\partial x} \right)$$

$$q_y \propto \rho_f \left(\frac{\partial H_f}{\partial y} \right)$$

In summary, if freshwater heads are used in a situation where the salinity field is stratified then the vertical hydraulic gradients may be exaggerated.

5.3 Aberg

The regional model by Svensson (1997) originally considered steady state flow in a single realisation of a randomly heterogeneous hydraulic conductivity field with two types of fluid conditions, freshwater (uniform-density) and a mix of freshwater and saltwater (variable-density). Although a single heterogeneous realisation results in a flow field that has an attractive spatial variability, the boundary conditions for the site-scale model would change if multiple realisations of the heterogeneous hydraulic conductivity field were used to describe the associated uncertainty, i.e., a stochastic approach.

For the purpose of the SR 97 project, the site-scale modelling of Aberg by Walker and Gylling (1998) was supplemented by a rerun of the regional steady state model by Svensson (1997) using a homogeneous hydraulic conductivity field and freshwater fluid conditions.

Given the different runs of the regional steady state model, there are several possible ways of transferring boundary conditions to the site-scale model. Walker and Gylling (1998) considered the following variants—

1. Use the freshwater heads of the regional model, which represents a homogeneous hydraulic conductivity field and a uniform-density fluid. This variant is referred to as the Base Case in Walker and Gylling (1998).

2. Use the pressure of the regional model, which represents a single realisation of a heterogeneous hydraulic conductivity field and variable-density fluid. Convert the resulting pressures to environmental heads[2].

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[2] Variable-density solutions cannot be used directly to provide boundary conditions to the site-scale model using HYDRASTAR, which assume uniform-density flow.

3. Use the freshwater heads of the regional model, which represents a single realisation of a heterogeneous hydraulic conductivity field and uniform-density fluid.
4. Avoid the concept of a regional model entirely and use instead the observed water table and sea level conditions as boundary conditions assuming uniform-density fluid. For this variant two sub-variants were treated—
    a) No flow conditions on all vertical sides and on the bottom side of the model domain.
    b) Hydrostatic head conditions on all vertical sides and a no flow condition on the bottom side of the model domain.

5.4 Beberg

Unlike the regional model of Aberg, the regional model of Beberg by Hartley et al. (1998) originally considered transient flow in a deterministically heterogeneous domain with transient boundary conditions and a variable-density fluid. For the purpose of the SR 97 project, the site-scale modelling of Beberg by Gylling et al. (1999a) was supplemented by a rerun of the regional model by Hartley et al. (1998). The rerun treated steady state flow with a uniform-density fluid.

The Base Case variant of the site-scale modelling of Beberg treated freshwater heads on all sides. As a variant, Gylling et al. (1999a) considered environmental heads instead of freshwater heads. The environmental heads were derived from the present-day solution for pressure using the original regional variable-density model.

5.5 Ceberg

The regional model of Ceberg by Boghammar et al. (1997) considered steady state flow in a deterministically heterogeneous domain with fixed boundary conditions and a uniform-density fluid. The site-scale modelling of Ceberg by Walker and Gylling (1999) focused entirely on uncertainties of the interior. The Base Case model treated freshwater heads on all sides and none of the variant simulations treated uncertainties in the boundary conditions.

6 CONCLUSIONS

Uncertainties in hydrogeological boundary settings should be looked into by means of sensitivity studies. In practical work this implies simulations with alternative processes, boundary conditions and even different sizes of the model domain. Generally speaking, however, most sensitivity studies dealing with groundwater flow focus on parameter heterogeneity mainly. The hydrogeological modelling performed in the SR 97 project constitutes an exception in this respect. Moreover, the SR 97 project contributes significantly to the study of nested numerical models, i.e., the numerical interplay between regional and site-scale numerical models. In particular, great efforts are made to address problems associated with (*i*) the telescopic mesh refinement (TMR) technique with regards to the stochastic continuum approach, and (*ii*) the transfer of boundary conditions between variable-density flow systems and flow systems that are constrained to treat uniform-density flow.

Regarding the regional hydrogeological modelling performed for the SR 97 project it may be concluded that the historical hydrogeological evolution is modelled differently at the three sites, although the overall handling is acceptable and in accordance with common modelling practice. For instance, at Aberg steady state variable-density flow is simulated, whereas at Beberg transient variable-density flow is simulated, and at Ceberg steady state uniform-density flow is simulated. At Aberg uncertainties in the size of the regional hydrogeological domain (RHD) and the type of boundary conditions are not examined. On the other hand, the size of the regional model domain at Aberg is very large, which probably puts the target area of interest sufficiently far away from the regional boundaries. At Beberg, the size, of the RHD is not varied but the lateral boundary conditions are modelled as dynamic in order to simulate the effect of changing groundwater conditions due to the post-glacial shore level displacement and subsequent variable-density flow. At Ceberg, steady state uniform-density flow is assumed while studying two different sizes of the regional hydrogeological domain as well as a number of different types of top boundary conditions.

The importance of taking variable-density flow into account is well demonstrated in the regional hydrogeological modelling performed at Aberg and Beberg. Both studies show that saline conditions may affect the location of discharge areas as well as the travel time calculations. The simulations of variable-density flow on the regional scale are based on pressure as a state variable, whereas the site-scale simulations in the canister defect scenario (CDS) of the SR 97 project are based on hydraulic heads and uniform-density flow. This study concludes that the efforts made to handle the uncertainties associated with this problem are satisfactory from a modelling point of view.

The regional modelling performed at Ceberg addresses the size problem by using two different sizes of the RHD. The results suggest that the smaller domain captures the body of the discharge areas found in the larger domain simulation. It may be noted, however, that at Beberg, which is comparable in size but modelled quite differently due to the presence of saline groundwater, the chosen RHD is shown to be too small in order to capture all of the discharge.

7 REFERENCES

Ahlbom, K., J.-E. Andersson, R. Nordqvist, C. Ljunggren,. S. Tirén and C. Voss (1991) Gideå study site, Scope of activities and main results, SKB TR-91-51, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Anderson, M. P. and W. W. Woessner (1992) *Applied Groundwater Modelling. Simulation of Flow and Advective Transport*, Academic Press, Inc., San Diego.

Andersson, J., K.-E. Almén, L. O. Ericsson, A. Fredriksson, F. Karlsson, R. Stanfors and A. Ström (1996) Important parameters to assess in geoscientific site investigations, SKB R-97-03, Swedish Nuclear Fuel and Waste Management Company, Stockholm, *in Swedish.*

Boghammar, A., B. Grundfelt and L. Hartley (1997) Investigation of the large scale regional hydrogeological situation at Ceberg, SKB TR-97-21, Swedish Nuclear Fuel and Waste Management Company

Cliffe, K. A., C. P. Jackson and S. T Morris (1995) Assessment model validity document; NAMMU: A program for calculating groundwater flow and transport through porous media, SKB AR-95-11, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Follin, S. (1992) Numerical calculations on heterogeneity of groundwater flow, SKB TR-92-14, Swedish Nuclear Fuel and Waste Management Company

Franke, O. L. and T. E. Reilly (1987) The effects of boundary conditions on the steady state response of three hypothetical ground-water systems - Results and implications of numerical experiments, USGS Water Supply Paper 2315, U.S. Geological Survey, Denver.

Gylling, B., D. Walker and L. Hartley (1999a) Site-scale groundwater flow modelling of Beberg, *in press*, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Gylling, B., M. Lindgren and H. Widén (1999b) Preparatory hydrogeological calculations for site scale models of Aberg, Beberg and Ceberg, SKB R-99-06, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Hartley, L. A. Boghammar, and B. Grundfelt (1998) Investigation of the large scale regional hydrogeological situation at Beberg, SKB TR 98-24, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Hedin, A. (1997a) Handling of data uncertainties in SR 97 calculations, SKB Internal PM 1997-04-10, Swedish Nuclear Fuel and Waste Management Company, Stockholm, *in Swedish.*

Hedin, A. (1997b) Premises for certain scenarios of SR 97, SKB Internal PM 1997-08-14, Swedish Nuclear Fuel and Waste Management Company, Stockholm, *in Swedish.*

Lusczynski, N. J. (1961) Head and flow of ground water of variable density, Journal of Geophysical Research, 66(12), 4247-4256.

Norman, S. (1992) HYDRASTAR – A code for stochastic simulation of groundwater flow, SKB TR-92-12, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Påsse, T. (1997) A mathematical model of past, present and future shore level displacement in Fennoscandia, SKB TR-97-28, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Saksa, P., and J. Nummela (1998) Geological-structural models used in SR 97, Analysis of uncertainties, SKB TR-98-12, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Spalding, D. B. (1981) A general purpose computer program for multi-dimensional one- and two-phase flow, Math. Comp. Sim., 8, 267-276.

Svensson, U. (1997) A regional analysis of groundwater flow and salinity distribution in the Äspö area, SKB TR-97-09, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Walker, D., I. Rhén and I. Gurban (1997) SR 97: Summary of hydrogeological conditions at Aberg, Beberg and Ceberg, SKB TR 97-23, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Walker, D. and B. Gylling (1998) Site-scale groundwater flow modelling of Aberg, SKB TR-98-23, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Walker, D. and B. Gylling (1999) Site-scale groundwater flow modelling of Ceberg, SKB TR 99-13, Swedish Nuclear Fuel and Waste Management Company, Stockholm.

Ward, D., D. Buss, J. Mercer and S. Hughes (1987) Evaluation of a groundwater corrective action at the Chem-Dyne hazardous waste site using a telescopic mesh refinement modelling approach, Water Resources Research, 23(4), 603-617.

Widén, H. and D. Walker (1998) SR 97 alternative modelling project: Stochastic continuum modelling of Aberg, *in press*, Swedish Nuclear Fuel and Waste Management Company, Stockholm.