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Assessment model validity document – HYDRASTAR: A stochastic continuum program for groundwater flow

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Abstract

The prevailing document addresses validation of the stochastic continuum model HYDRASTAR designed for Monte Carlo simulations of groundwater flow in fractured rocks. Here, validation is defined as a process to demonstrate that a model concept is fit for its purpose. Preferably, the validation is carried out by comparison of model predictions with independent field observations and experimental measurements. In addition, other sources can also be used to confirm that the model concept gives acceptable results. One method is to compare results with the ones achieved using other model concepts for the same set of input data. Another method is to compare model results with analytical solutions.

The model concept HYDRASTAR has been used in several studies including performance assessments of hypothetical repositories for spent nuclear fuel. In the performance assessments, the main tasks for HYDRASTAR have been to calculate groundwater travel time distributions, repository flux distributions, path lines and their exit locations. The results have then been used by other model concepts to calculate the near field release and far field transport.

The aim and framework for the validation process includes describing the applicability of the model concept for its purpose in order to build confidence in the concept. Preferably, this is made by comparisons of simulation results with the corresponding field experiments or field measurements. Here, two comparisons with experimental results are reported. In both cases the agreement was reasonably fair. In the broader and more general context of the validation process, HYDRASTAR results have been compared with other models and analytical solutions. Commonly, the approximation calculations agree well with the medians of model ensemble results. Additional indications that HYDRASTAR is suitable for its purpose were obtained from the comparisons with results from other model concepts. Several verification studies have been made for HYDRASTAR and referenced here. In addition, the system of tools to present and inspect input and output data is shortly described in this document.

HYDRASTAR is developed to produce probabilistic input to other models in the SKB model chain PROPER, which has been used in performance assessment studies conducted by SKB. As for most model concepts there are advantages and limitations for HYDRASTAR. However, one conclusion is that HYDRASTAR is valid for its purpose, i.e. local-scale stochastic groundwater modelling and advective transport for performance assessments under fresh-water conditions.

Sammanfattning

Föreliggande dokument behandlar validering av den stokastiska kontinuum modellen HYDRASTAR som har konstruerats för Monte Carlo-simuleringar av grundvattenflöde i sprickigt berg. Validering definieras här som en process för att demonstrera applicerbarheten av en modell för dess syfte. Det är att föredra att valideringen utförs genom jämförelser mellan modellprediktoner och fältobservationer samt oberoende experimentresultat i så stor utsträckning som möjligt. Dessutom kan andra källor användas för att säkerställa att modellkonceptet ger acceptabla resultat. En metod är att jämföra med resultat från andra modellkoncept vid användande av samma uppsättning data. En annan metod är att jämföra modellresultat med analytiska lösningar.

Modellkonceptet HYDRASTAR har använts i ett flertal studier av förvarsfunktioner för hypotetiska förvar för använt kärnbränsle. I dessa säkerhetsbedömningar har den huvudsakliga uppgiften för HYDRASTAR varit att producera fördelningar av gångtider, fördelningar av specifikt grundvattenflöde vid förvarsdjup, banlinjer och utströmningsområden. Resultaten har sedan använts i andra modellkoncept för att beräkna närzonsutsläpp och transport genom fjärrzonen.

Syftet och ramverket för modellvalidering inkluderar att beskriva modellkonceptets applicerbarhet på det den är avsedd för och att bygga förtroende för konceptet. Om möjligt, görs detta genom att jämföra simuleringsresultat med sammanhörande fältexperiment eller mätningar i fält. Här är två jämförande fall med experimentella resultat rapporterade. I båda fallen överensstämmer resultaten relativt hyggligt. I ett bredare och mer generellt perspektiv av valideringsprocessen, har HYDRASTAR-resultat jämförts med andra modellkoncept och analytiska lösningar. Vanligtvis har god överensstämmelse med analytiska approximationer uppnåtts för medianvärden av ensemlestatistik. Ytterligare indikationer på att HYDRASTAR är tillämplig för dess syfte erhålls i jämförelserna med andra modellkoncept. Ett flertal verifieringsstudier har gjorts för HYDRASTAR och är refererade här. Dessutom är ramverket av verktyg för att presentera och kontrollera indata och utdata kortfattat beskrivet i dokumentet.

HYDRASTAR är utvecklad för att ge probabilistiska indata till andra modeller i SKB:s modellkedja PROPER, som har använts i flera säkerhetsanalyser utförda av SKB. HYDRASTAR har fördelar och nackdelar som de flesta modellkoncept. Emellertid är en slutsats att HYDRASTAR är möjlig att använda för sitt syfte, dvs. stokastisk grundvattenmodellering och advektiv transport för säkerhetsanalyser i lokal skala och under färskvattenförhållanden.

Contents

1 Introduction

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/. As part of the SKB 91 Project the code was applied successfully to the Finnsjön site, /Norman, 1992a; SKB, 1992/. The code also has been used in simulations of field experiments and modelling studies, e.g. simulations of the Long-term Pumping and Tracer Test (LPT2) performed at Äspö HRL /Walker et al, 1996/, and in the comparative Alternative Modelling Project, AMP, /Selroos et al, 2001/. Furthermore, the code was used in the SR 97 Project /SKB, 1999/ for modelling of three sites arbitrarily denoted Aberg, Beberg and Ceberg /Walker and Gylling, 1998; Gylling et al, 1999a; Walker and Gylling, 1999/ using data from Äspö HRL, Finnsjön and Gideå, respectively.

Starprog AB developed and tested the code under contract to SKB, beginning in 1989 /Norman 1991, 1992a/. Various authors have contributed to the development and testing of the code, most notably /Norman, 1991, 1992a/, /Morris and Cliffe, 1994/, /Lovius and Eriksson, 1993, 1994/, /Walker et al, 1997/ and /Walker and Bergman, 1998/. A set of test cases is available to confirm that every new development is compatible with earlier versions. The test cases 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 current version, 1.7, 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 /Norman, 1992a/ based on /Moye, 1967/. 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 in space and an implicit multistep method in time to create linear systems of equations. A pre-conditioned 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, flow field, the travel paths and arrival times for advected contaminants /SKB, 1996/.

Similar to validation documents written for other model concepts, such as NAMMU /Cliffe et al, 1998/ and COMP23 /Romero et al, 1995/, validation is here defined as a process of building confidence in the simulation tool. Comparing simulation results with measured values from field experiments is probably the most important issue in the validation process. Since large-scale field experiments are scarce other sources can also be used to build confidence in the model concept. One method is to compare results with the ones achieved using other model concepts for the same set of input data. Comparison with analytical solutions is another way to check that the model is doing what it is designed for. The latter is often included in the process of verification, i.e. checking that the used numerical method is handling the underlying mathematical equations correctly. Support and documentation on how to use such an expert code as HYDRASTAR are two important components to avoid simulation mistakes and obtain trustworthy results. To document and to handle developments, the use of a source code control system is required to fulfil quality assurance.

1.1 Organisation of the document

In section 2 the validation framework for this report is described. The aim and meaning of the word validation is defined within this context. Other issues for the confidence building such as model verification, comparisons with analytical solutions and comparisons with other model concepts are included.

In section 3, the stochastic continuum concept, which is the base for HYDRASTAR is briefly described. In addition, the basic mathematical equations for this concept and the numerical methods to solve them are included.

Section 4 gives examples of studies where HYDRASTAR have been used. The studies include two comparisons with available field experiments and measurements. Performance assessments and other simulation studies where HYDRASTAR have been applied are also described. In this section, model verification, comparisons with analytical solutions, and comparisons with other model concepts are also included.

Section 5 gives the framework for quality assurance, support, documentation, development, and source code control. All these issues are important to obtain reliable results in modelling.

Finally a Summary and discussion section are included. Here, the subjects dealt with in this report are summarised followed by a discussion.

2 Validation framework

In the literature there are different definitions of validation. Here, the meaning of validation is adopted from the field of performance assessments of repositories for nuclear waste, e.g. the work of validating NAMMU /Cliffe et al, 1998/. In that report the key issue is to build confidence in NAMMU. Quoting /IAEA, 1988/, the authors write that the definition most appropriate for the NAMMU validation is:

"Validation is a process carried out by comparison of model predictions with independent field observations and experiment measurements. A model cannot be considered validated until sufficient testing has been performed to ensure an acceptable level of predictive accuracy over the range of conditions over which the model may be applied. (Note that the acceptable level of accuracy is judgmental and will vary depending on the specific problem or question to be addressed by the model.)"

The NAMMU report includes descriptions and references to comparisons with field observations. In addition, the model concept, model development, and model verification, in the context of checking that the model correctly represents the mathematics it is based on, are thoroughly described. The authors define their distinction between validation and verification. Verification is the process of establishing confidence that the program correctly solves the mathematical equations, which it encapsulates, whereas validation is the process of building confidence in the models themselves and their applicability to the physical situation under consideration. This is also in agreement with the updated glossary from /IAEA, 1993/.

The code COMP23 calculates the near field release from a possible canister failure. It is originally based on the code NUCTRAN /Romero, 1995/. To be used for performance assessments within the PROPER package, the code was slightly modified, mainly for input and output handling, but not in a conceptual meaning. For use in the model chain PROPER the code is denoted COMP23. The model validation report for NUCTRAN mainly describes the model concept. It is probably difficult to set up experiments for validation of this code to test all capabilities of the model. Hence, no attempt to validate the code against experiments has been made. Validation is defined in the same way as for NAMMU. However, there is a short section about model verification by comparisons with analytical solutions and by comparisons with an independent code. The comparisons are briefly discussed and the reader is referred to publications. It should be noted that in a verification study by /Gould et al, 1996/, NUCTRAN is tested against two other models.

For HYDRASTAR, the ambition of the prevailing validation document is to use the same definition of validation as above. In general terms, validation can be described as the process of building confidence in the fitness of purpose of models that are used in performance assessment and hence in the results obtained from the models. The aim of validation in the context of performance assessment should be to demonstrate that the model is adequate for the purpose for which it is intended.

Preferably, validation in this context is made by comparisons of model predictions with results from field experiments. Since there are not many experiments conducted in the local scale, typical in the order of kilometres, which HYDRASTAR is designed for, the confidence building has to be based on other issues as well. In this report, model verification, comparisons with analytical solutions, and comparisons with other model concepts are also included.

In the following section, the stochastic continuum concept, which is the base for HYDRASTAR, is briefly described. In addition, the basic mathematical equations for this concept and the numerical methods to solve them are included. For the available field experiments a section is written. Performance assessments and simulations studies using HYDRASTAR are included. A section gives the framework for quality assurance, support, documentation, development and source code control.

3 Model concept

The objective of the HYDRASTAR program is to perform Monte Carlo simulations in order to solve the stochastic hydrology equation:

$$\nabla (K(x)\nabla h(x,t) = S_s(x)\, \partial h(x,t)/\partial t - q(x,t) \tag{1}$$

with boundary conditions

$$h(x,t) = h_1(x) \text{ for } x \in \partial C_1 \tag{2}$$

$$\partial h(x,t)/\partial n = 0 \text{ for } x \in \partial C_2 \tag{3}$$

and initial condition

$$h(x,t_0) = h_0(x) \text{ for } x \in C \tag{4}$$

where $K(x)$ is a given stochastic function equal to the hydraulic conductivity field and h is the hydraulic head. $S_s(x)$ is the specific storativity and $q(x,t)$ is a source term. To treat the stationary problem (time independent), equation (1) is solved, with the right hand side equal to zero, i.e. no source term $q(x,t_0)$ is needed to describe the stationary problem handled in HYDRASTAR, together with boundary conditions (2) and possibly (3).

The computational domain, C, i.e. the domain in which the above equation is assumed to be valid, is always a parallelepiped in the three dimensional space. The main reason for this restriction is to decrease computational demand of the code meant to function in Monte Carlo fashion. Also the great uncertainty on subsurface heads or groundwater fluxes makes the positioning of the boundaries of a computational domain less important. The well defined natural boundaries set by geology and topography beyond the local HYDRASTAR are honoured by a regional model coupled to the local model boundaries. By taking the values of the hydraulic head on the boundary from a regional computation of the hydraulic heads one achieves head conditions similar to reality which are of Dirichlet type (equation (2), where h_1 is a given function and ∂C_1 is standard notation for (part of) the boundary of C). In this version of HYDRASTAR Neumann boundary condition equation of no flow type (3) may also be used (n is the normal to the boundary). Note that a well-posed problem requires Dirichlet boundary condition on at least one part of the boundary.

The input stochastic model is given in terms of the log transformed conductivity field

$$Y(x) = \log 10\ (K(x)) \tag{5}$$

which is assumed to be a normally distributed random function. Commonly, the stochastic model is based on field data and then inferred into HYDRASTAR. In a trivial calculation the conductivity field may satisfy a stationary expectation value, but that is seldom the case in realistic simulations. For example, fracture zones and depth zones are often included in the computational domain as trend functions. The stochastic model for this log conductivity can be given in two different fashions.

A first alternative is to specify a trend function $E\,[Y\,(x)]$ and a covariance function for the residual process

$$E\,[Y'(x)\;Y'(z)] = C(x - z) \qquad (6)$$

where $Y'(x)$ is a standard notation for the residual process i.e.

$$Y'(x) = Y\,(x) - E\,[Y\,(x)] \qquad (7)$$

and $E\,[\,\cdot\,]$ is standard notation for the expectation value operator.

A second alternative is to avoid the need to specify the trend functions by only assuming that the expectation of the log conductivity is constant in a neighbourhood of each point. These so-called *kriging neighbourhoods* are further discussed in /Norman, 1992b/. This alternative involves conditioning on field data.

To perform simulations using HYDRASTAR, it is emphasised to infer field data and/or interpretations of field data into the model. The coupling of field data to the stochastic differential equation above is achieved by the following steps:

First the stochastic model for the conductivity field $K(x)$ is derived from the actual measurements. Secondly, the actual conductivity measurements themselves and their positions could be used to condition the simulations. In addition, the conductivity field can also be conditioned on measured heads. For this an inverse technique is used, where the conductivity in pilot points are calibrated to make the differences between computed and measured heads as small as possible. Rock domains and fracture zones may be inferred as trends in the conductivity field.

3.1 Generation of the conductivity field

In order to represent a site in HYDRASTAR, in addition to boundary conditions, an interpretation of the hydraulic properties must be inferred. There are two main methods to achieve that. One method is to explicitly include distributions of conductivity for the prescribed model domains. The other method is implicit and uses conditioning on data. Both methods are however based on observed field data.

The explicit method involves inference of a geostatistical model of the rock property hydraulic conductivity based on borehole data. Commonly such a geostatistical model contains interpreted properties as a mean conductivity for the rock mass and a mean conductivity for each fracture zone. This implies also that the geometry of each domain is determined and that the domains may be included into the model as trend functions. The geostatistical model also contains the variance of the conductivity and the correlation length. A semivariogram is commonly created in the geostatistical analysis. The semivariogram can then be converted into a covariance model.

The implicit method includes letting HYDRASTAR condition the conductivity field based on borehole data. The latter method needs information on the rock mass, variance in conductivity and correlation length, in addition to borehole data in HYDRASTAR format. In this implicit method to include trends in data, the concept of ordinary kriging neighbourhoods is used. 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).

The analysis is based on the hydraulic conductivity measurements. In general these are performed on different scales, that is using different packer intervals. Commonly the conductivities are interpreted from field measurements of pressure and flux histories in packed off sections pumping tests of sample bore holes using the formula of /Moye, 1967/. The flow field model that inspired this formula has been honoured in the algorithm for regularisation (upscaling) of the conductivities from the scale of the measurement sections to the computational model cell dimensions /Norman, 1992a/. Trends (i.e. spatial dependency of the expectation value) in the conductivity data may be included implicitly through the use of ordinary kriging neighbourhoods or prescribed explicitly for specific regions.

In addition, it is possible to infer a nugget effect. Several authors have noted that the spatial correlation of hydraulic conductivities commonly exhibits such small-scale variability, referred to as a nugget effect /La Pointe, 1994; Birgersson et al, 1995/. The nugget effect can be viewed as a microscale variance, e.g. a linear, independent contribution to the total variance in conductivity due to uncorrelated measurement error. Previous versions of HYDRASTAR only had options for covariance models with perfect correlation at zero separation distance. Work was made by /Walker et al, 1997/ to implement and test an option to allow the specification of a nugget effect.

If a depth dependency in the hydraulic properties is interpreted from the field data, it is possible to include this in the model domain. The depth dependency of conductivity may be included by specifying a power function or a step function. For repository performance assessment purposes, a simplified geometry of tunnel systems may be included together with their possible effect on the modelled conductivity field.

The hydraulic properties of the model domain are specified by using an algorithm in the code to generate the conductivity field. In the current version of HYDRASTAR, 1.7, the Turning Bands algorithm /Journel and Huijbregts, 1978/ is used to generate realisations of the hydraulic conductivity field, optionally conditioned on the observed hydraulic conductivities.

3.2 Solution of hydrology equation

3.2.1 Spatial discretisation

In HYDRASTAR the spatial discretisation of the hydrology equation (1) is carried out by using a finite difference approximation on a staggered mesh. That is a mesh where the node representation of different entities does not coincide, i.e. one set of nodes represents the hydraulic head and another set represents the hydraulic conductivity. For this type of representation, the Darcy velocity is defined as:

$$\mathbf{v} = -K(r)\nabla h(r,t)) = -\begin{bmatrix} Kxx & Kxy & Kxz \\ Kyx & Kyy & Kyz \\ Kzx & Kzy & Kzz \end{bmatrix} \begin{bmatrix} \partial h/\partial x \\ \partial h/\partial y \\ \partial h/\partial z \end{bmatrix} \tag{8}$$

The left-hand side of the hydraulic equation (1) may now be written:

$$\nabla \bullet (-\mathbf{v}) = \mathrm{div}(-\mathbf{v}) = -\frac{\partial v_x}{\partial x} - \frac{\partial v_y}{\partial y} - \frac{\partial v_z}{\partial z} \tag{9}$$

In the isotropic case, the off diagonal elements of the conductivity tensor are zero. Hence three scalar equations are obtained:

$$v_{\xi} = -K_{\xi} \frac{\partial h}{\partial \xi}, \quad \xi = x, y, z \tag{10}$$

which are approximated by finite differences. The staggered mesh formulation means that two sets of computational nodes are obtained. One set represents the scalar hydraulic head values and the possible source terms at the centres of parallelepipeds (mass balance elements). The other intermediate set represents the components of the velocity and conductivity at the midpoints of the faces of the parallelepipeds. From each head node in the interior of the computational domain *C* there are six conductivity nodes connecting to six neighbour head nodes in 3D.

Imposing the boundary conditions, a coupled linear system of equations for the heads in the stationary case is obtained. The conductivity matrix is sparse, at most six off-diagonal elements per row, and symmetric negative definite; properties which are utilised in the solution process.

In case of transient computations the time derivatives in equation (1) will generate a diagonal storativity matrix, and a coupled linear system of ordinary differential equations has to be integrated in time.

3.2.2 Time discretisation

For the integration in time of the space discretised transient hydrology equation (1), with boundary and initial conditions, the MOLCOL (Modified One-Leg COLlocation) family of methods is used /Dahlquist, 1983/. This is a family of implicit multistep methods, which includes the famous BDF methods (e.g. BDF-1 or backward Euler method) and, for linear problems, theta methods (e.g. Crank Nicolson method) as special cases.

The HYDRASTAR implementation of the MOLCOL method /Lovius and Eriksson, 1994/ uses a predictor-corrector procedure choosing the order of the difference scheme and size of the time step to minimise the computational work with the constraint that the local truncation per step is smaller than a specified tolerance. This is particularly important in simulating this kind of systems where there is a wide range of time scales present due to the discretisation of the space operator and the varying conductivity field.

An implicit method with good stability properties, such as a BDF method of order one or two, with step size control allows larger and larger time steps as the rapid changes die out.

3.2.3 Solution of linear systems of equations

The linear system of equations, arising from the discretised stationary hydrology equation or from the transient hydrology equation within each time step, is large and sparse. Also, since the matrices of these linear systems are symmetric and definite, this suggests the use of some other method than a direct solver. In HYDRASTAR a semi-direct method is used based on a Conjugate Gradient method /Golub and van Loan, 1989/ with preconditioning. With Conjugate Gradient (CG) methods applied to this type of problem the solution converges quite fast, especially if the initial guess is good as it is when using prediction by extrapolation in the time steps of the transient integration.

3.3 Calibration

The purpose of the calibration is to utilise also steady-state head measurements and transient head histories, recorded during transient interference tests where water is pumped in packed off sections of boreholes, to improve the realisation of the hydraulic conductivity field. Doing this means that an inverse problem has to be solved, i.e. determine a hydraulic conductivity field of the hydrology equation from measured hydraulic heads.

3.3.1 Calibration technique

An inverse problem, such as calibration of hydraulic conductivity fields, is in general ill-posed. However it can be made computationally tractable by suitably restricting the high-frequency content in the degrees of freedom of the allowed hydraulic conductivity field. In the inverse technique implemented in HYDRASTAR /Eriksson and Oppelstrup, 1994/, proposed by RamaRao and LaVenue /RamaRao et al, 1995/, this is done by letting the hydraulic conductivity in strategically chosen pilot points be the degrees of freedom in the calibration. The hydraulic conductivity in the pilot points are to be chosen to minimise the error between the simulated and observed hydraulic heads.

The pilot points are included as conditioning data in the geostatistical simulation so that the influence by the pilot points is determined by the range of the spatial correlation and the choice of kriging neighbourhood. That is, the influence of the adjustments is governed by the range of the input variogram model, decreasing with distance from the pilot point. An additional larger-scale effect arises from the influence of the pilot points on the mean of the ordinary kriging neighbourhood. If the input hydraulic conductivity field to the calibration is conditioned on observed hydraulic conductivities, we arrive at a hydraulic conductivity field conditioned on both the observed hydraulic conductivities and the measured heads. This consequently increases the reliability of the hydraulic conductivity field, and reduces the uncertainty in subsequent simulations.

Briefly the calibration means finding the pilot point conductivities that minimise the objective function, a weighted sum of squares of head errors for all head measurement locations and all times. This is done by a Conjugate Gradient method /Polak and Ribiere, Numerical Recipes, 1986, 1989/ with line search, where the gradients are computed by solving the adjoint state equation. The line search in a CG iteration uses a search direction, being a combination of gradient and old search direction, and fits a second order polynomial by evaluating the objective function at some locations along line and then finds the minimum of that polynomial. The line search is where much of the computational effort lies since every evaluation of the objective function means a time integration of the hydrology equation.

Finally, a remark on initial and boundary conditions in connection with calibration on drawdowns, i.e. changes relative initial steady-state heads, is made. Assuming that time independent Dirichlet boundary conditions and Neumann boundary conditions (with prescribed flow) are appropriate for our specific problem, then the drawdowns satisfy homogeneous boundary conditions, i.e. the original boundary conditions but with zero values for both heads and flows (the explicit values only effect the initial steady-state). This means a simpler problem can be solved when calibrating on just drawdowns: Choose a zero initial steady-state head field (no computation needed) and use the homogeneous versions of the boundary conditions when integrating. No explicit knowledge of how the heads and flows vary along the boundary, just the type of boundary conditions, is needed.

3.4 Particle tracking

The transport modelling in HYDRASTAR is done by calculating stream lines and groundwater travel times to the boundaries in the resulting velocity fields. In general the interesting results are exit locations and travel times to the surface and not to the vertical boundaries and bottom boundary of the computational domain. To deal with this problem HYDRASTAR uses an extended domain.

3.4.1 Solution of stream line equation

To calculate stream lines and groundwater travel times the streamline equation has to be solved, i.e. the velocity has to be found and integrated. Within the computational domain (the outermost mass balance elements excluded) the velocity field is obtained from the solution of the stationary hydrology equation, the simulated conductivity field and the flow porosity. The velocities in the conductivity nodes are then interpolated using trilinear interpolation, which generates a continuous velocity field. Outside this domain the velocity field is predicted by a simplified kriging method using velocities in kriging neighbourhoods of the computational domain /Norman, 1992b/. For the integration a 4'th order Runge-Kutta /Dahlquist and Björk, 1974/ method is used.

4 Confidence in the model

The prime goal of model validation is to build confidence in the model concept. In other words, does the model predict groundwater flow and possible transport in fractured rock adequately to be used in repository performance assessments? Are the results reasonable for the type of modelling tasks the model is designed for? Preferably, validation in this context is made by comparisons of model predictions with results from field experiments. Since there are not many experiments conducted in the local scale, typical in the order of kilometres, which HYDRASTAR is designed for, the confidence building has to be based on other issues as well. In this section, model verification, comparisons with analytical solutions, and comparisons with other model concepts are also included.

4.1 Applications of the model

HYDRASTAR has been used in several performance assessments of hypothetical repositories at the site-scale. In most cases boundary conditions from a regional model have been used. The main tasks for HYDRASTAR have been to produce groundwater travel time and repository flux distributions, path lines and exit locations for the path lines. The results have then been used by other models to calculate the near field release and far field transport. Exit locations can be used in the biosphere modelling.

4.1.1 Simulations of field experiments

Model validation by comparisons of field measurements and simulation results are exemplified by two studies. In one study, the Long-term Pumping and Tracer Test is simulated. In the other, measured heads from boreholes are compared to HYDRASTAR results.

Simulation of the Long-term Pumping and Tracer Test (LPT2)

A stochastic groundwater modelling study was performed by /Walker et al, 1996/ for the second Long-term Pumping and Tracer Test (LPT2) using HYDRASTAR. The experiment was conducted at the Äspö Hard Rock Laboratory (HRL), which is an underground research facility located near the Oskarshamn nuclear power plant on the east coast of Sweden.

Various investigations have taken place at Äspö before, during and after construction of the laboratory. This included a tracer test and a number of interference pumping tests that were later analysed as training and calibration exercises for the numerical models of the site. A major test of this kind was the second Long-term Pumping and Tracer Test (LPT2) conducted in the autumn of 1990. The pumping phase lasted for three months and was combined with a large-scale converging tracer test. Although the simulation study incorporates data obtained during the construction phase, the simulations are of events which occurred prior to the construction of the HRL.

Unlike previous modelling studies of the LPT2, this study used the inverse modelling capabilities of HYDRASTAR to condition the model results to the observed hydraulic heads /Walker et al, 1999/. The purpose of this conditioning via inverse modelling is to improve the reliability of input hydraulic conductivity fields and thus minimise the uncertainty of the model predictions. Preliminary simulations evaluated the boundary conditions, grid extent and grid density, all of which were restricted by the computational demands of a larger domain and by code limitations. The preliminary simulations also indicated that the model is quite sensitive to changes in specific storativity and kriging parameters. The final calibrated model simulations were successful in representing the response of the rock mass to the LPT2. Specifically, the mean of the Monte Carlo realisations of simulated drawdowns generally reproduced the magnitude, timing, and shape of the observed drawdowns. The observed drawdowns generally were bracketed by an interval of plus or minus one standard deviation from the mean of the realisations. This indicates that the ensemble of realisations has bracketed the true characteristics of the HRL, supporting both the conceptual model and its representation by HYDRASTAR. However, some discrepancies in the magnitude and timing of the observed versus the simulated drawdowns were revealed at several locations, such as the upper sections of one borehole. A comparison of experimental values with simulation results from an un-calibrated case is shown in Figure 4-1.

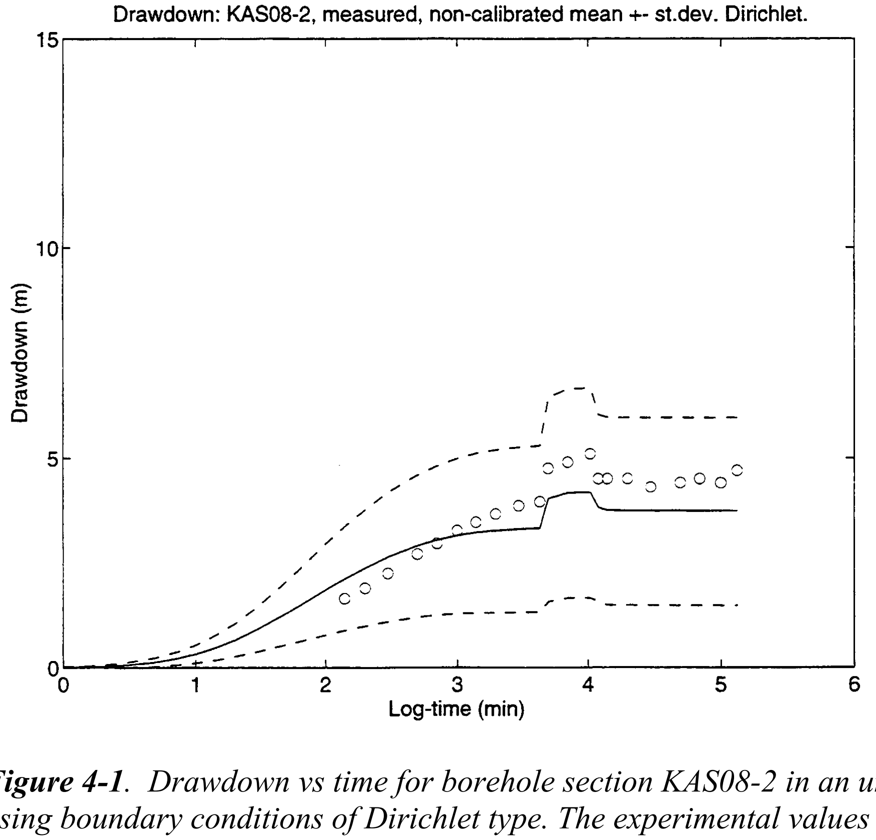

***Figure 4-1**. Drawdown vs time for borehole section KAS08-2 in an un-calibrated case using boundary conditions of Dirichlet type. The experimental values are symbolised with small rings, the median of simulation results is plotted as a line and median +/– one standard deviation are drawn as dashed lines /Walker et al, 1996/.*

Comparison of simulated and measured heads in boreholes

The Safety Report 97 study (SR 97) is a comprehensive performance assessment illustrating the results for three hypothetical repositories in Sweden /SKB, 1999/. In support of SR 97, hydrogeologic modelling of the hypothetical site called Aberg, which adopts input parameters from the Äspö Hard Rock Laboratory, was performed /Walker and Gylling, 1998; Walker et al, 2001/. The study used HYDRASTAR to compute the heads, Darcy velocities at each representative canister position and the advective travel times and paths through the geosphere.

In this study a nested modelling approach was used, with a deterministic regional model providing boundary conditions to a site-scale stochastic continuum model. The model was 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 addressed uncertainties in the inference of parameters and the boundary conditions.

To validate the results, observed heads from boreholes at Äspö were compared to 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 4-2 presents the Base Case simulated versus observed heads at locations corresponding to representative borehole sections at the site.

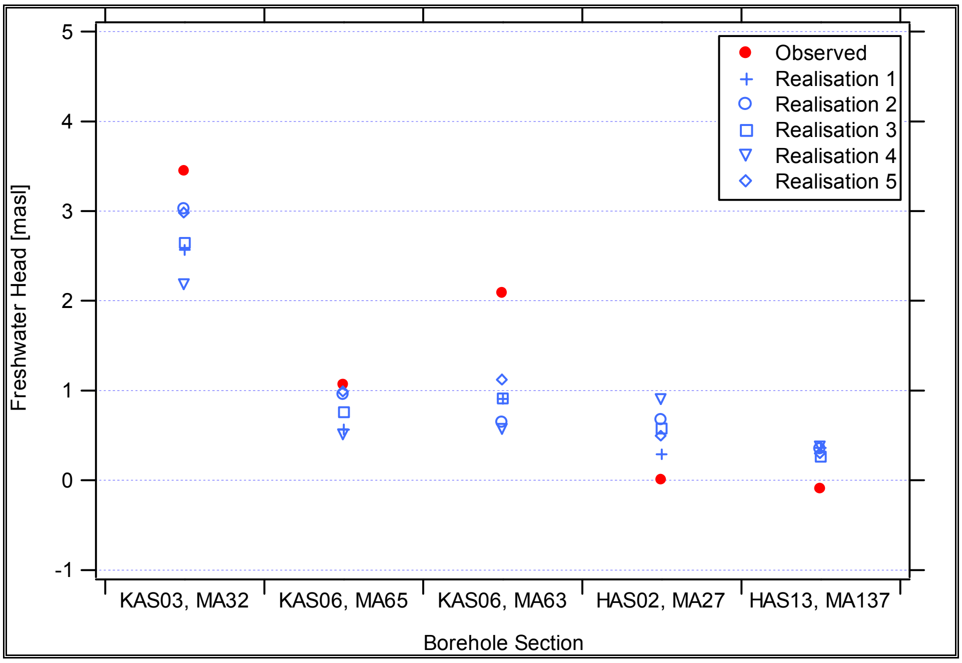

***Figure 4-2.** Observed and simulated freshwater heads for five realisations of the Aberg Base Case /Walker and Gylling, 1998/.*

Because this is a Monte Carlo study of heterogeneous fields, each realisation will not exactly match the observed data. Based on a analysis of the errors, the maximum error of observed versus model simulated heads should be approximately 2.0 m. The heads of five realisations presented in Figure 4-2 are generally within this error, suggesting that the model-simulated heads agree with the observed heads.

4.2 Verification of the model

In this context, verification is the process of verifying that the mathematical equations formulated for the model concept are correctly solved by the numerical methods within the code. In the following section comparisons of HYDRASTAR results with analytical solutions and other models are described.

4.2.1 Comparison with analytical solutions

Prior to the process of setting up a model in HYDRASTAR it is common to estimate performance measures of a site, such as groundwater travel time and flux at repository level, using an analytical solution based on Darcy's law. These types of approximation uses average properties of the rock, assumed flow paths and flow porosities, and estimated values of the gradient.

For Aberg in the SR 97 study, an approximate calculation of the travel time from repository depth to the surface was performed as a check on the validity of the model. 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. Based on 100 realisations with 120 path lines each, the model results suggest that the median travel time was 10 year for a flow porosity, ε_f, of $1x10^{-4}$.

The same type of comparisons between analytical results and model results were also made for Beberg and Ceberg within SR 97. Both in the approximate calculation and in the HYDRASTAR simulations, a flow porosity of $1x10^{-4}$ was used. For Beberg, the approximate calculations showed that the travel times should be between 20 to 70 years depending on starting position. The median of the ensemble results for the 100 realisations of the Beberg Base Case indicated a median travel time of 56 years.

The rock mass and fracture zones of the Ceberg site in SR 97 are less conductive compared to the other two sites. The approximate calculations of the Ceberg site suggested that the travel times should be on the order of 1000 years, which is roughly in agreement with the 100 realisations of the Ceberg Base Case where the median travel time is 1700 years.

HYDRASTAR verification studies

In a report by /Norman, 1991/ verification of HYDRASTAR is addressed by using comparisons with an analytical approximation and a test case designed for the international project HYDROCOIN /NEA/OECD/SKI, 1988/. The analytical approximation is based on a perturbation solution /Neuman et al, 1987/ of the stationary case of Equation 1. Variograms of the conductivity and head values are compared with the corresponding analytical approximations. The results show some resemblance, but are not fully satisfactory according to Norman. By using a finer mesh the results are improved. However, in the comparison with HYDROCOIN, the results are more favourable. This comparison with other model results is described in a section below.

In a study made by /Morris and Cliffe, 1994/ a set of verification tests are carried out on the HYDRASTAR code. The tests have been designed to complement and extend the verification work carried out by /Norman, 1991/. Some of the tests computed by Morris and Cliffe are summarised in the following text.

In one test, the case of uniform mean flow at small variance of the logarithm of hydraulic conductivity was considered. In this test, the grid is 1000x1000x0.1 m represented by 121x121x4 nodes, i.e. basically a 2D case, and the variance in the hydraulic conductivity field is about 0.2 in $\log_{10}$. There is an analytical solution for the first and second order moments of velocity and for the particle displacements in this case /Dagan, 1989/. Calculations carried out using HYDRASTAR to solve this problem were compared with the analytic results. The agreement was found to be satisfactory. In particular, the moments of particle displacement are in very good agreement with those obtained by Dagan. Since this type of calculation uses most of the numerical and statistical functions of the code, this test indicates that HYDRASTAR is capable of calculating accurately both the flow and transport in two-dimensional flows with small variance of the logarithm of hydraulic conductivity /Morris and Cliffe, 1994/.

Another test concerned the same type of problem as above, except that the variance is no longer small. In this case there is no valid analytical solution and so the results obtained with HYDRASTAR were compared with the two-dimensional code SPV2D, developed by AEA Technology. The results of HYDRASTAR and SPV2D were found to be reasonably consistent. However, a number of numerical difficulties were encountered, which may be overcome by refining the mesh and performing more realisations to obtain a stable solution.

The final part of the study by /Morris and Cliffe, 1994/ concerned the case of uniform flow in three dimensions at small variance. In this test, the model domain is 666x666x666 m represented by 41x41x41 nodes, and the variance in the hydraulic conductivity field is again 0.2 in $\log_{10}$. As in the two-dimensional case an exponential covariance model was inferred. Calculations carried out using HYDRASTAR to solve this problem were compared with the analytic solution for the second order moments of the particle displacements /Dagan, 1989/. The agreement was found to be satisfactory. In particular, the moments of particle displacement are in good agreement with those obtained by Dagan. This is shown in Figure 4-3. Again this indicates that HYDRASTAR is capable of calculating accurately both the flow and transport in three-dimensional flows with small variance of the logarithm of hydraulic conductivity.

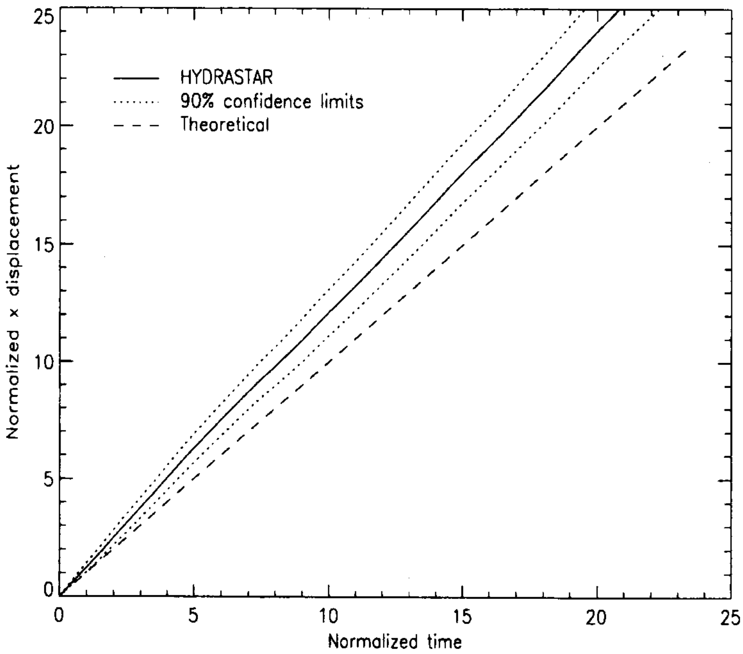

Figure 4-3. *Plot of the normalized longitudinal displacement as a function of normalized time, for the case of two-dimensional flow and small variance of the logarithm of hydraulic conductivity /Morris and Cliffe, 1994/.*

4.2.2 Comparison with other models and test cases

HYDRASTAR was used in the SR 97 study to model three hypothetical sites Aberg, Beberg and Ceberg. These sites take their data from the Äspö HRL, the Finnsjön site, and the Gideå site, respectively. In another study, the site Fjällveden was modelled using HYDRASTAR. Prior to the HYDRASTAR simulations, all of these sites have been modelled by using other model concepts, different domains, and different scales, which gives an opportunity to compare HYDRASTAR results to the other models' result.

Prior to the SR 97 HYDRASTAR Aberg simulations, /Svensson, 1997/ determined the advective travel times from –450 masl to ground surface for the Äspö site. Using a nonuniform flow porosity with an average of $\varepsilon_f = 4x10^{-3}$, Svensson found that 15% of the particles would have reached the surface after 100 years. Although Svensson's model used spatially variable flow porosity, the results can be roughly rescaled to a flow porosity of $\varepsilon_f = 1x10^{-4}$ 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 the SR 97 study are roughly comparable to those of /Svensson, 1997/.

In the SKB 91 study of the Finnsjön site, /SKB, 1992/ examined advective travel times from a hypothetical repository in the Northern block using a similar modelling approach as in the SR 97 Beberg study. In both the SKB 91 and SR 97 studies, HYDRASTAR was used for the local scale. The SKB 91 study found a median travel time of approximately 100 years, longer than the 56 years of the Beberg Base Case of the SR 97 study. In the SKB 91 study, approximately 50% of the stream tubes failed to reach the upper model surface in contrast to the 0.7% that failed in this study. Several differences between the approaches used by these studies contribute to the differences in the results. One difference between the studies is that the SKB 91 regional study used a Dirichlet (constant head) upper boundary condition at the groundwater table surface. The regional NAMMU model of the SR 97 study used a Dirichlet upper boundary at ground surface elevation and a coarser finite element mesh, both of which may contribute to differences in gradients and recharge patterns. SKB 91 and this study also differ in the representation of hydraulic conductivity.

The SR 97 site Ceberg took its data from Gideå. In a modelling study of the Gideå site, /Carlsson et al, 1983/ determined the advective travel times from –500 depth to ground surface. Using a flow porosity of $\varepsilon_f = 4 \times 10^{-3}$, they found that the travel times ranged from 1000 to 300,000 years. Although the range of their results is extreme, the results of the Carlsson et al. study suggest that the travel times of the SR 97 Ceberg study are reasonable.

The Alternative Modelling Project, AMP

The Alternative Modelling Project (AMP), conducted by SKB, evaluates uncertainties regarding the conceptualisation of water conducting features in models of groundwater flow and solute transport for fractured crystalline rock /Selroos et al, 2001/. The AMP applies three alternative modelling approaches to flow and transport in fractured media: stochastic continuum (SC), discrete fracture network (DFN), and channel network (CN). Each of these alternatives have been applied successfully to field-scale experiments in fractured rocks /Walker et al, 1996; Uchida et al, 1994; Gylling, 1997/, but it is possible that their results might have important differences when applied to performance assessment (PA). The AMP evaluates the impacts of these alternative approaches on the performance assessment of a hypothetical deep geologic repository for high-level nuclear waste. An original motivation for the AMP study was to assess the degree of conservatism and/or limitations of adopting the SC approach as the chief flow modelling approach in the SR 97 project /SKB, 1999/.

Three separate modelling teams participated in the AMP /Dershowitz et al, 1999; Gylling et al, 1999b; Widén and Walker, 1999/, each experienced in the use of their models and familiar with the site hydrogeology of Aberg. The hypothetical site Aberg adopts input data from Äspö HRL. The problem premises and the compilation of results are explicitly specified so that the comparison will illustrate the impacts of alternative modelling approaches rather than the impacts of different hydrogeologic interpretations.

The alternative approaches yield similar exit locations for path lines, medians for travel time and canister flux, suggesting that the problem premises (boundary conditions, major conductors, etc) dominate the results. This further suggests that the choice of groundwater flow conceptual model had little impact on expected repository performance in the present application. Figure 4-4 presents the performance measure medians and the ranges of 5th and 95th percentiles.

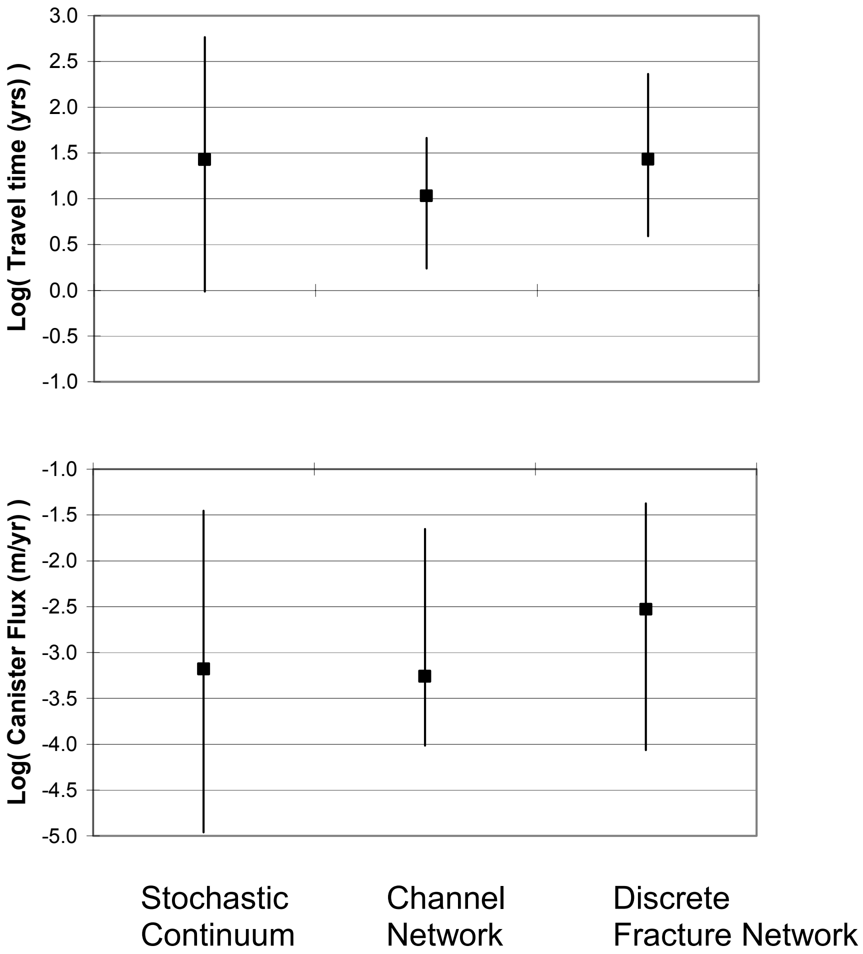

Figure 4-4. *Performance measures for the three alternative approaches to the Aberg repository. Median (squares) and range as 5th and 95th percentiles (whisker).*

Figure 4-4 indicates that the SC approach yields the largest performance measure ranges. The reasons for the difference in the measure ranges are several. Among the most important are model strategy and interpretation of data. However, the range of the SC results suggests that, for these performance measures, using the SC approach alone is conservative with respect to PA in the present application.

HYDROCOIN

One of the cases in the test examples for HYDRASTAR is taken from the international project HYDROCOIN /NEA/OECD/SKI, 1988/, which was an international effort for comparison and verification of different groundwater computer codes. The test example adopts its data from the two-dimensional Case 2 of Level 1 within HYDROCOIN. The case involves steady state flow in a rock mass intersected by permeable fracture zones. The test case was designed to test the capabilities of different codes to handle large permeability contrasts. In the HYDRASTAR test examples, this case verifies the finite difference solver and the particle tracking algorithm.

Calculations on two different meshes were performed, one with coarse resolution and another with finer resolution. The finer mesh reproduces these values better, which gives results with a larger span between the highest and lowest head value for each depth. In general the results are in good agreement with the other teams' results, except for a small offset, around +3 m, in the head values. The offset is due to the used approximation of the top boundary values /Norman, 1991/. This could be overcome by choosing a more sophisticated way of representing the top boundary than the approximation used in these calculations. For the path line modelling it was observed that the ability to resolve the fracture zones depends on the resolution of the mesh. However the path line results are in general consistent with the other model results.

Comparison with NAMMU

Supplemental regional simulations using the finite element concept NAMMU, based on the Beberg regional groundwater model of /Hartley et al, 1998/, were performed within SR 97. These simulations are performed to supply the site scale modelling with appropriate boundary conditions. Boundary conditions for the HYDRASTAR Base Case and three variants were obtained. Statistics for the travel time (t_w) and initial Darcy velocity (q_c) for each of the regional models corresponding to the site-scale variants were calculated. These statistics are based on a small sample (16) of start locations distributed uniformly in the Northern Rock block. Hence, the results presented are approximate, and intended for broad comparison with the more detailed site-scale transport study. For the Base Case, the results compare favourably. Mean travel times and initial Darcy velocities of the regional model are within one standard deviation of the site-scale model. The regional minimum and maximum values also compare well with the 5th and 95th percentile, respectively, of the site-scale models.

In another study, the finite element concept NAMMU was used to simulate the site Beberg at local-scale /Marsic et al, 2000/. As mentioned, NAMMU was previously used to simulate Beberg, but then at the regional scale /Hartley et al, 1998/. In the deterministic local-scale NAMMU modelling study, the same model domain and boundary conditions were used as in a deterministic variant of the SR 97 HYDRASTAR calculations. In an attempt to make the models as similar as possible, the actual conductivity field from HYDRASTAR was imported and converted to NAMMU format. The results from NAMMU show great resemblance to the HYDRASTAR results. Especially, the distribution of flux at repository level for the starting positions is very similar. The median flux at repository level is higher just by a factor of 1.06 for NAMMU than for HYDRASTAR. Path lines and exit locations reveal some minor differences. This is expected though, since small local differences in the representations of the conductivity field may cause discrepancies in the path lines. The exit locations for both HYDRASTAR and NAMMU are shown in Figure 4-5. The median travel time is longer by a factor 2.5 for NAMMU than for HYDRASTAR. At first, this may seem to be a quite large difference, but the path line calculations are very sensitive to variations in the heterogeneous conductivity field. In /Marsic et al, 2000/ the differences in results and model concepts are thoroughly analysed. Mainly, the differences are explained by different numerical discretisation techniques, and different path line algorithms used in the two models. Due to the difference in model concepts it is difficult to avoid that the grid properties, such as conductivities and heads, are not perfectly matched in space. If the conditions at the starting positions are not identical in the two models it may lead to

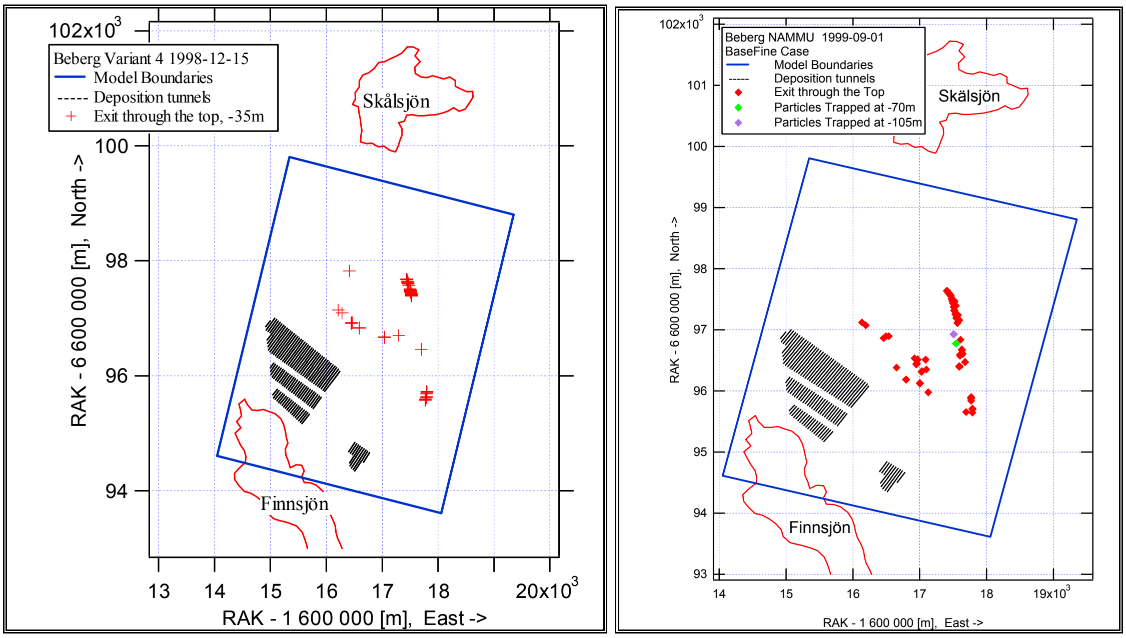

Figure 4-5. *Calculated exit locations for Beberg, in the deterministic HYDRASTAR Variant 4 to the left and in the corresponding NAMMU case BaseFine to the right. For both models the results are for one realisation of 120 starting positions. (RAK is a Swedish national metric coordinate system).*

larger discrepancies in the travel time results than the differences in the repository flux results. Both the HYDRASTAR and the NAMMU calculations are deterministic. It is possible that the difference between the model results might decrease for a set of stochastic simulations.

4.3 Pre- and post-processing of results

There are several options available for pre- and post-processing of input and output data for HYDRASTAR. One option to study that the shape and location of fracture zones are the expected is to use the application HYDRAVIS /Hultman, 1997/ built on the commercial visualisation package AVS Explorer. HYDRAVIS is an interactive graphical processor for HYDRASTAR, permitting users to view the repository layout, deterministic zones, hydraulic conductivities, stream tubes, and hydraulic heads in 3D. An example of that is shown in Figure 4-6a,b. Visualisations of fracture zones can then be combined with visualisation of tunnels and hence a visual inspection of that the location of starting positions in relation to fracture zones are the expected. This is also verified by the routine TRAZON in HYDRASTAR which checks for each starting position if it is in a fracture zone or in the rock mass.

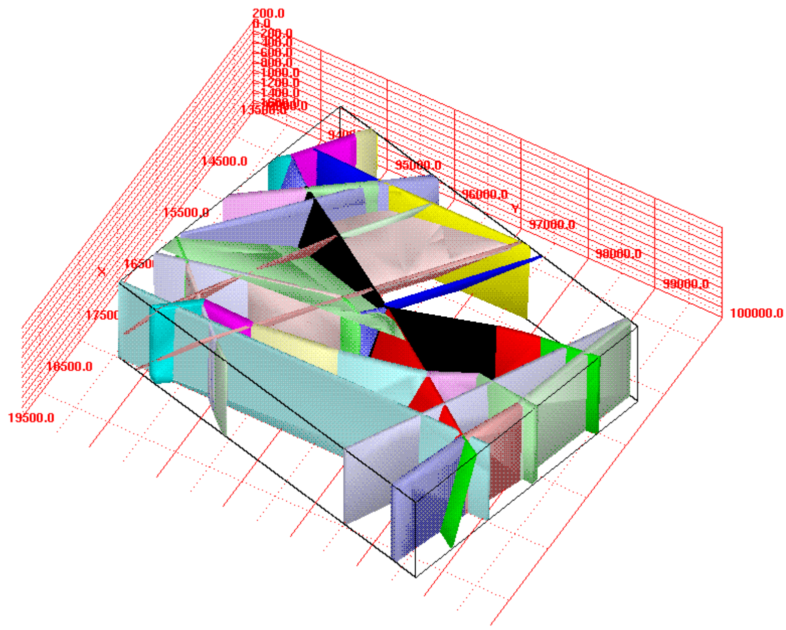

__Figure 4-6a.__ HYDRASTAR representation of Beberg conductive fracture zones in an isometric view from northeast.

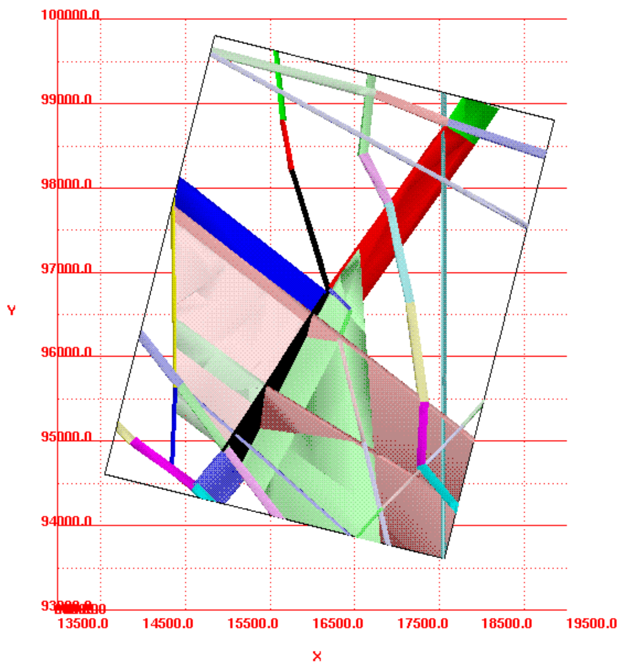

__Figure 4-6b.__ HYDRASTAR representation of Beberg conductive fracture zones in a plan view from above.

The generated conductivity fields and calculated head fields can also be visualised in HYDRAVIS. By visual inspection it is then possible to see if e.g. a fracture zone leaves the expected traces in the conductivity field. This is shown in Figure 4-7 for a deterministic case using the same fracture zone geometry as above. Tunnels at the repository level are shown as dashed lines. In addition, it is possible to verify that the geostatistical model given as input to HYDRASTAR is generated for the whole domain or parts of the domain.

Commonly, the flow balance over the boundaries of the model domain is produced in a simulation study using HYDRASTAR. This is done by specifying the domain to study in the input data and then post-process the output data with the program BC-FLUX. The second step is optional and simply aids the presentation of results. The obtained HYDRASTAR flow balance can then be used to check that the numerical solution is accurate enough and that is in agreement with that the regional model produced for such cases.

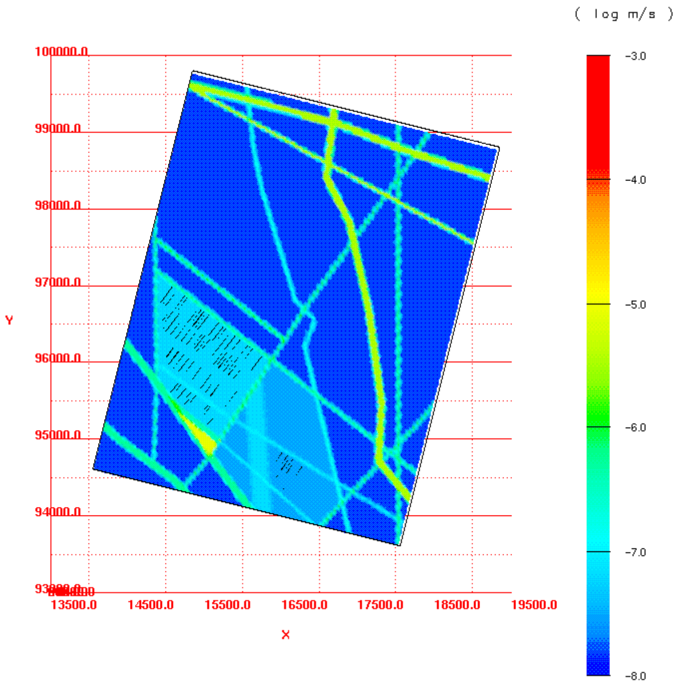

Figure 4-7. *Log$_{10}$ of hydraulic conductivity on a plane cutting through repository level in Beberg Variant 4 (deterministic representation of hydraulic conductivity).*

Tools for statistical post-processing have been developed based on Statistica and Matlab by Kemakta Konsult AB. Not only are the tools helpful in the process of presenting simulation results, but also can they be used to interpret simulation results. By studying the ensemble statistics or individual canister locations deviations from the expected outcome can be detected. An example of graphical presentation of ensemble statistics is shown in Figure 4-8.

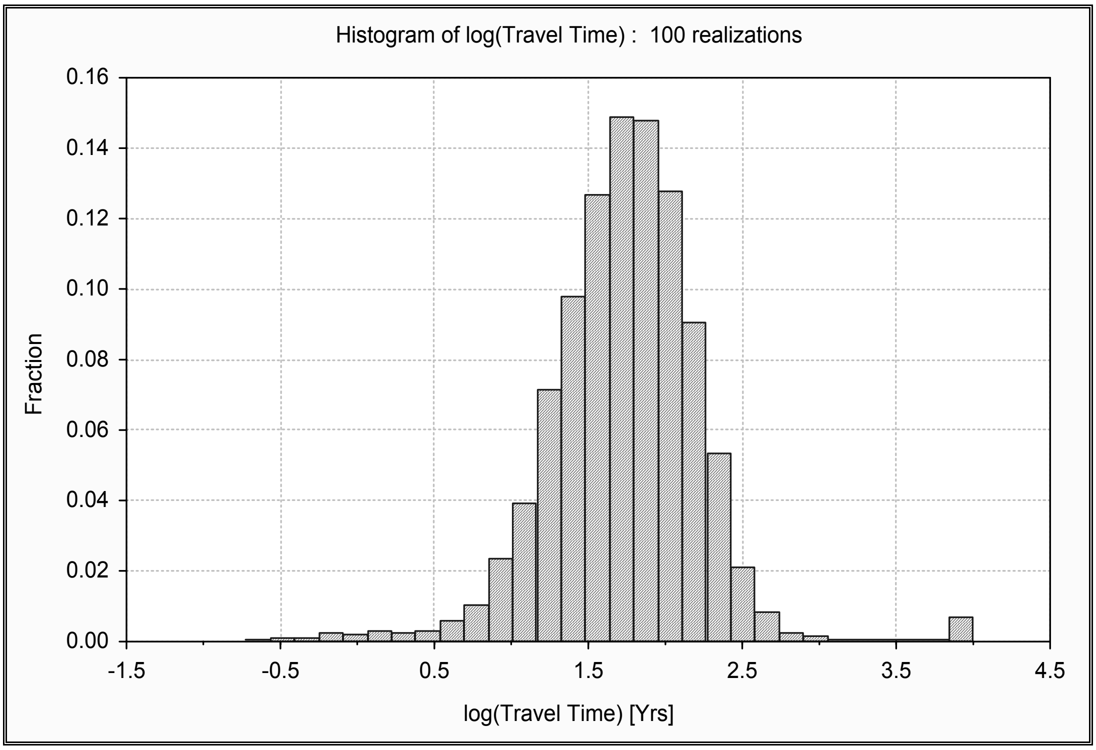

Figure 4-8. *Relative frequency histogram of log_{10} travel time for Beberg Base Case. Results for 100 realisations of 120 starting positions and a flow porosity of $\varepsilon_f = 1x10^{-4}$.*

5 Documentation and code administration

During the performance assessments and model studies by using HYDRASTAR and other models, a framework has been developed for quality assurance and peer review. This includes to document and test model developments, and to store the source code in a control system. Another, important issue is to provide support and documentation on how to use the code. Traditionally, input data and results are documented. Commonly, the modelling studies are exposed to internal and external review.

5.1 Documentation and publications

A number of documents are available on various applications of the code, e.g. /Walker and Gylling, 1998/. There is a User's Guide /Gylling and Lovius, 2001/ on how to use HYDRASTAR available both on paper and on-line. The Programmer's Guide details the routines of the code and the organisation of the code /SKB, 1994/. Updates of the code are reported in technical documents and then made available e.g. in the User's Guide.

Applications of HYDRASTAR are documented in SKB reports, e.g. /SKB, 1992, 1999/. For performance assessments conducted by regulatory demands, the studies are reviewed by the Swedish Nuclear Inspectorate (SKI). In the case of SR 97, the review was aided by the /OECD, 2000/.

In order to obtain other possibilities for review, condensed performance assessments and other modelling studies can be published in scientific journals and presented at international conferences. For example, the PA for Aberg, Beberg and Ceberg is summarised in the Hydrogeology Journal /Walker et al, 2001/ and the Alternative Modelling Project has been presented at the conference Fractured Rock 2001 and is summarised in Journal of Hydrology /Selroos et al, 2001/. Other publications are included in the section References.

5.2 Source Code control

The development of HYDRASTAR is under strict control using the Unix Source Code Control System (SCCS). This means that it is possible to keep track of every modification and to come back to an earlier version if that is needed. Based on SCCS there is a build environment available for the developer. The build environment enables that the developer works with a copy of the newest code version. A new development can then be checked by running the available test cases. If the new development passes the test examples, the main source code is updated and the modification is documented.

5.3 Development using test cases

A number of test cases have been set up for HYDRASTAR in the test batch denoted *testhydra*. The tests cover various features of HYDRASTAR ranging from normal steady state calculations to transient simulations. One important objective of the test batch is to provide tests to be run after a code modification and hence verify that the new version is giving the expected results. After a code modification is made, the test batch should be executed to check that results are the same as prior to the modification of the code. By running the test batch several different features of the code are tested. The test batch /Widén, 1996; Gylling and Lovius, 2001/ contains examples that can be compared with analytical solutions, an example from the literature, HYDROCOIN /OECD, 1983/, a transient simulation, and cases from performed performance assessments.

Summary and discussion

HYDRASTAR has been used in several performance assessments of hypothetical repositories at the site-scale. In most cases boundary conditions from a regional model have been used. The main tasks for HYDRASTAR have been to produce groundwater travel time and repository flux distributions, path lines and exit locations for the path lines. The results have then been used by other models to calculate the near field release and far field transport. Exit locations can be used in the biosphere modelling.

The aim and framework for the validation process includes building confidence in the applicability of the model concept for its purpose. Preferably, this is made by comparison of simulation results with corresponding field experiments or measurements. In the broader and more general context of the validation process, model results can be compared with other models. In addition, checking model results with analytical approximations is good modelling practice. By using the features in HYDRASTAR, results can be monitored regarding representation of the used geostatistical model, obtained boundary flow balance and verification on localisation of particle starting positions in relation to e.g. fracture zones. Model input data and results can be checked by visualisation e.g. by using HYDRAVIS. Tools for statistical analysis are commonly used to present model results, but also to check that the results are reasonable, and to help the interpretation of the results.

Model validation by comparison of field measurements and simulation results are exemplified by two studies. In one study, the Long-term Pumping and Tracer Test is simulated. In the other, measured hydraulic head from boreholes are compared to HYDRASTAR results. In both cases the agreement was reasonably fair. Comparisons of HYDRASTAR results with analytical approximations have been made frequently. Commonly, the approximation calculations agree well with the medians of ensemble results. Additional indications that HYDRASTAR is suitable for its purpose include several comparisons with results obtained by using other model concepts. In a study made by /Morris and Cliffe, 1994/ a set of verification tests are carried out on the HYDRASTAR code. The tests have been designed to complement and extend the verification work carried out by /Norman, 1991/, and helped to build confidence that the code will produce correct results when applied to realistic cases.

In a performance assessment it is important to document not only the results, but also the used input data for quality assurance. Preferably, the modelling studies are reviewed by expertise in the field. Another important issue is to provide support and documentation on how to handle the code. It is of advantage to have an experienced modelling team to ensure the credibility of the results. Model developments should be documented and tested, and the source code should be stored in a source code control system. These issues are not just valid for HYDRASTAR, but modelling in general. However, the performance assessments carried out by using HYDRASTAR have been performed under these premises.

As mentioned HYDRASTAR has been used for groundwater flow modelling in several performance assessment studies conducted by SKB. The model is developed to produce input to other models in the SKB model chain PROPER. It is relatively easy to infer a geostatistical model based on standard methods from the hydrogeolical literature. It seems like the stochastic continuum concept, which HYDRASTAR is based on, has reached a certain level of acceptance in the field of modelling of flow and transport in fractured rock. Other concepts may however give a more realistic representation of the transport in the fractured rock. As for all codes there are some limitations in HYDRASTAR and possible improvements to do if it is considered necessary. For example, HYDRASTAR does not include transient simulations due to fluid density effects, hydraulic anisotropy is approximated with stochastic anisotropy, path lines are simulated as stream tubes i.e. no dispersion due to a heterogeneous flow field, and the path line algorithm is purely advective. However, interactions between species and the rock, and radioactive decay are handled by another concept within the model chain PROPER for the far-field tracer transport calculations.

There are other codes available that may be used to overcome the limitations in HYDRASTAR, if the situation demands that. Codes that have been used by SKB to calculate flow and transport in fractured rock include e.g. FracMan, NAPSAC, CHAN3D, NAMMU and DarcyTools. FracMan /Dershowitz et al, 1999/ and NAPSAC /Hartley et al, 1998/ are based on discrete fracture network concepts. CHAN3D /Gylling, 1997/ uses a channel network approach to simulate flow and transport. NAMMU is based on a continuum-porous-media approach /Cliffe et al, 1998/. DarcyTools (including the hydraulic conductivity generator GEHYCO) is based on transforming a discrete fracture network into a continuum representation /Svensson, 1999/. Even if another more advanced concept is to be used in future performance assessments, HYDRASTAR may play a role in the verification process and produce results as reference. However, one conclusion of this document is that HYDRASTAR is valid for its purpose, i.e. groundwater modelling for performance assessments within the SKB framework.

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