

Site investigation SFR

**Hydrogeological modelling at SFR
using DarcyTools**

Site description SFR version 0.0

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April 2009

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Abstract

The general purpose of this study is to provide an opportunity for the modelers to gain experiences and knowledge of the specific problems and challenges associated to the SFR repository before new data will be available. One important objective is also to test the confidence in DarcyTools modeling. This is done by setting up a DarcyTools model as similarly as possible to a previous model set up in the numerical code GEOAN /Holmén and Stigsson 2001/.

This study has demonstrated a number of typical obstacles encountered in transferring a hydrogeological model from one numerical code to another. These obstacles involve tracking previous data versions and simplifications made in the numerical implementation, and precludes preserving the model intact in the transfer process. Nevertheless, the modeling results agree rather well, particularly for open repository conditions.

On important conclusion from the study is that the water divides should be studied in more detail – and if needed – revise the model domain accordingly. Another improvement to the next model version (SFR v.0.1) would be to use a rotated coordinate system and also to update the algorithm for calculating inflow/outflow to a saturated tunnel in DarcyTools.

Sammanfattning

Det övergripande syftet med denna modelleringsövning (version 0.0) är att ge modelleringsteamet inom Projekt SFR-utbyggnad chansen att bekanta sig med specifika problem och utmaningar inom projektet innan nya data blir tillgängliga. En viktig uppgift är också att testa tilltron till modelleringsverktyget DarcyTools. Detta görs genom att sätta upp en modell i DarcyTools med liknande parameterisering som användes i en tidigare modellering i koden GEOAN /Holmén and Stigsson 2001/.

Övningen visar att det finns ett antal svårigheter med att överföra en hydrogeologisk modell från en numerisk kod till en annan. Till exempel svårigheter med att få tag på gamla data och förenklingar som användes i den tidigare modellen vilket förhindrar en korrekt överföring från en modell till en annan. Trots det redovisar de olika modellerna snarlika resultat, speciellt för öppet förvar simuleringarna.

En viktig slutsats från simuleringarna är att de framtida vattendelarna som använts för att definiera modellområdet behöver studeras mer detaljerat och eventuellt uppdateras inför nästa modellversion. Andra förbättringar inför nästa version skulle också vara att rotera koordinatsystemet och uppdatera algoritmen som beräknar inflöde/utflöde till vattenmättade tunnlarna i DarcyTools.

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1.1 Objectives

The hydrogeological model has a central role in this project: to improve the understanding and characterization of the surrounding hydrogeologic system. More precisely, three tasks have been formulated for the hydrological modeling work:

- 1) provide feedback to the ongoing site investigation,
- 2) test and evaluate different engineering design cases, and
- 3) deliver flow paths (or groundwater flow distribution) for the subsequent safety assessment.

As a first step, a hydrological model version 0.0 will be set up in DarcyTools /Svensson et al. 2008/ using “old” SFR data available before the site investigation started in April 2008. This approach will create a possibility for the modelers to gain experiences and knowledge of the specific problems and challenges associated to the SFR repository before new data will be available.

The objectives of model version 0.0 are as following:

1. Test confidence in DarcyTools modeling. If a DT model is set up as similarly as possible to a previous model set up in the numerical code GEOAN /Holmén and Stigsson 2001/, can “old simulations” be reproduced using “old data”?
2. Simulate the open repository conditions and calibrate skin/grouting to match recorded tunnel inflow.
3. Predict flow in backfilled tunnels and the evaluation of flow paths with time at steady state conditions.
4. Test if it is possible to run transient simulation, that is, release particles at 2000 AD and follow the particles for each time step up to 5000 AD.

1.2 Sequence of work

First, the model in DarcyTools will be set up as similarly as possible to the previous model, described in /Holmén and Stigsson 2001/. Then the hydraulic properties, grouting and skin will be calibrated to reproduce measured inflow to the repository during operational phase (i.e. open repository).

The calibrated model will then be used to predict flow in tunnels and flow paths at steady state conditions for the following times: 2000, 3000, 4000 and 5000 AD. The model will also be used to test if it possible to produce transient flow trajectories.

2 Site description

2.1 The SFR repository

A layout of the repository is given Figure 2-1. The tunnel system consists of different access tunnels, four deposition tunnels (BMA, BLA, BTF1 and BTF2) and a silo (SILO). The deposition area is located approximately 50 meters below the seabed. The layout of the SFR repository is available as CAD files, which are imported into DarcyTools. Different CAD-files corresponds to different tunnel sections.

2.2 Model setup

One of the objectives with this study is to compare model results between DarcyTools and the GEOAN model /Holmén and Stigsson 2001/. Therefore the hydraulic 0.0 model version of the SFR repository is set up as similarly as possible to the previous model, described in /Holmén and Stigsson 2001/. The most significant differences between the two model setups are:

- 1) topographical data used, i.e. Digital Elevation Models (DEMs),
- 2) model domain,
- 3) top boundary conditions applied,
- 4) the discretisation of the model domain into a computational mesh,
- 5) the regional DZ-model.

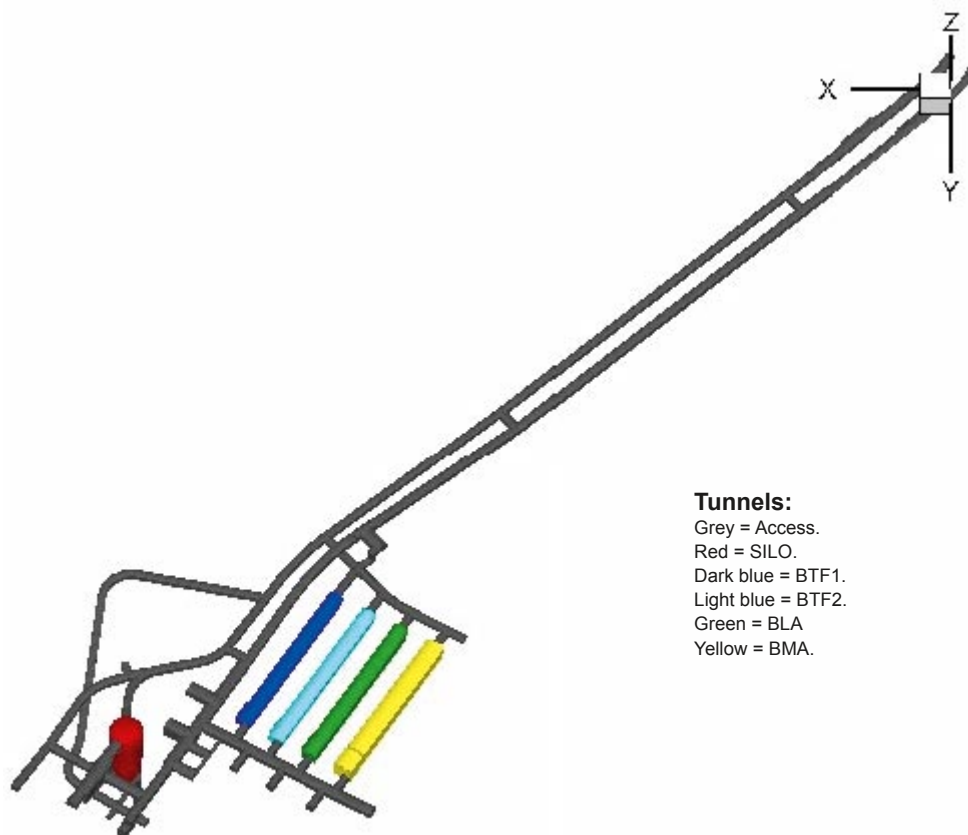


Figure 2-1. Layout of the SFR repository. North is in the Y-direction.

The reason for using a different Digital Elevation Model was that the old DEM is now unavailable. The most important difference between the two DEMs is that the ridge above the repository was not included in /Holmén and Stigsson 2001/. The local domains (i.e. target volumes) are almost identical in the two model setups. However, the enclosing catchment domains (model domain) differ somewhat. The reason for this is that the outer lateral boundaries will be assigned no-flow conditions, and in order to do so, it is more accurate to define these boundaries by local surface water divides. This difference is expected to have insignificant influence of the model result. Different top boundary condition was used simply because the two models use different algorithms for calculating the top boundary condition. A higher discretisation of the computational mesh was used in DarcyTools partly because it is possible with the computer capacity available today. But also, DarcyTools uses an unstructured Cartesian grid system which makes it possible to have a higher resolution surrounding geometrical objects (i.e. tunnels), which can be read in as CAD-files.

2.2.1 Model domain

The lateral flow boundaries of the model follow local surface water divides except for the north-east boundary. Instead, the north-east boundary is following a trench in the topography, this is to ensure that a sea level will be present at 5000 AD. The size of the model was chosen large enough to minimize boundary effects in the vicinity of the SFR repository and the model extends down to 800 m depth below the datum plane (RHB 70). Figure 2-2 illustrates the model domain together with the topography and the present day shoreline.

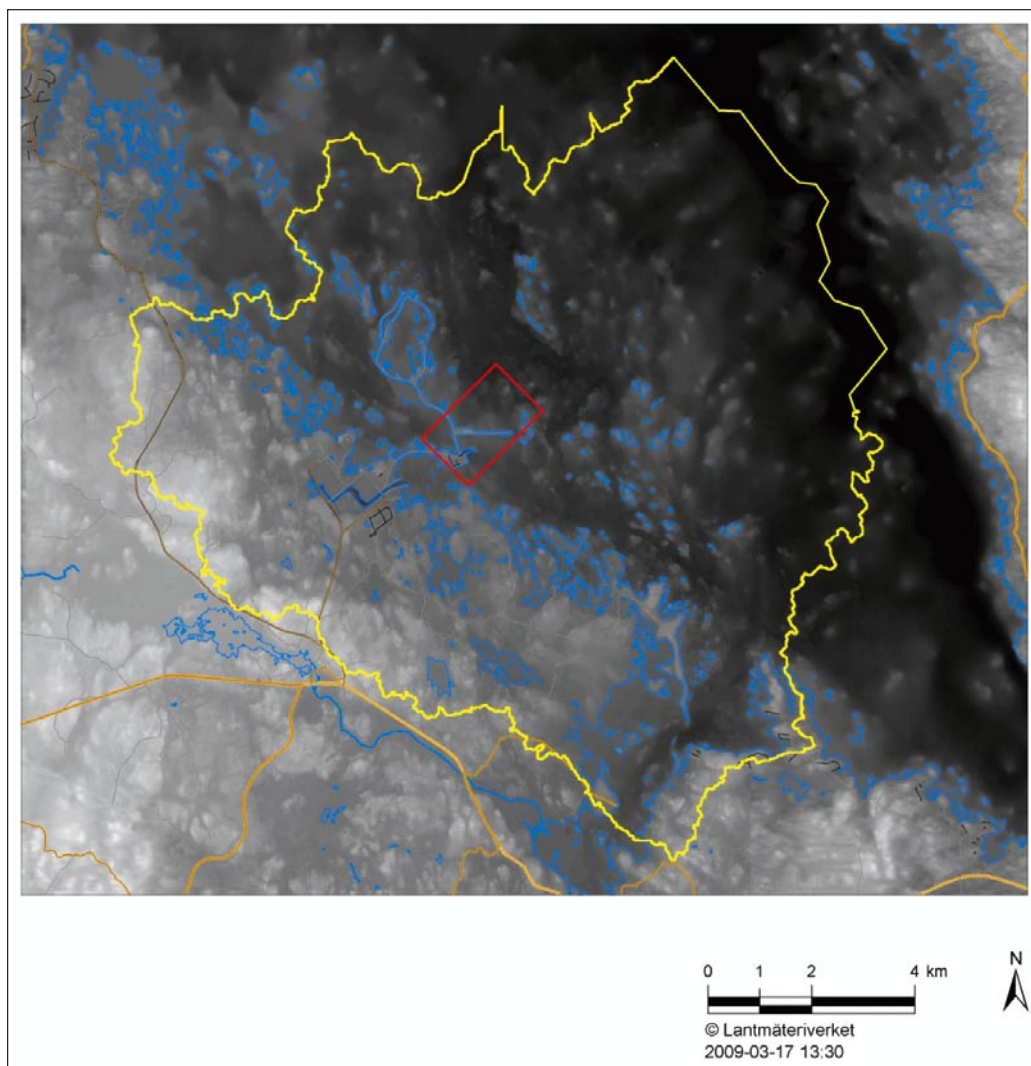


Figure 2-2. The yellow line represents the regional model domain for the hydro model version 0.0, the red line the local model domain for SFR version 0.0 and the blue contour the shoreline at 2000 AD.

The surface topography of the model domain is taken from the latest DEM with a horizontal spatial resolution of 20 m /Strömberg and Brydsten 2008/, which is not the same as the one used in /Holmén and Stigsson 2001/. To circumvent artificially large effects of the ridge above the SFR repository, its topography was constrained so as not to exceed -1 meter above sea level. That is, in the model the ridge is cut off at 1 m depth below the datum plane (RHB 70).

The local model domain for SFR version 0.0 is roughly the same as the domain used for the local model in /Holmén and Stigsson 2001/. The extent of the local model domain for SFR version 0.0 is shown together with the local deformation zones in Figure 2-3.

2.2.2 Geology

Two different scales are considered in the model. The local model domain for version 0.0 (Figure 2-3) is modeled in high detail and referred to as the local scale. This local scale domain is surrounded by a regional scale domain, which is modeled in less detail, e.g., includes only deformation zones exceeding 10 km of length, and has a coarser discretisation (Figure 2-4). The local domain resolves deformation zones to a higher level of detail (using a lower cut-off of 300 m for deformation zones). Consequently, the effective conductivity of rock mass will be lower within the local domain than on the regional scale (where rock mass is defined as the fractured rock not resolved by deformation zones; i.e. HRD definitions following notation by /Rhen et al. 2003/).

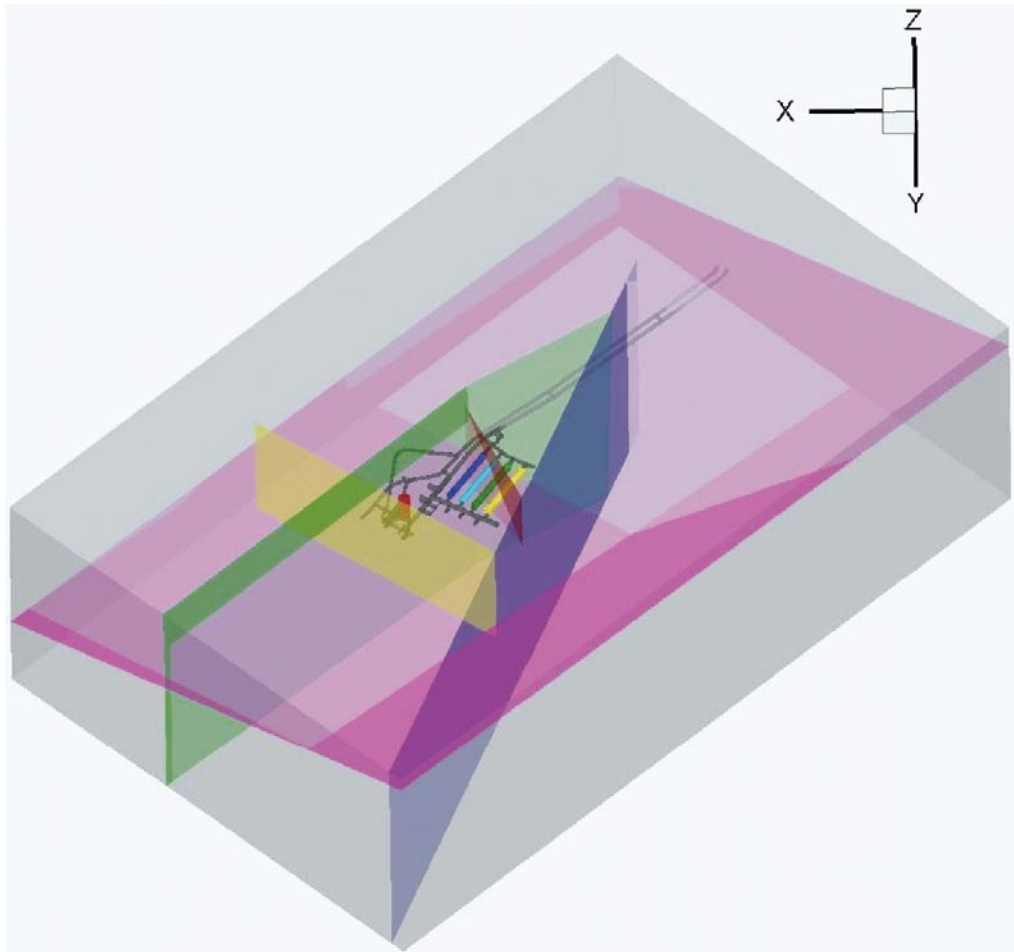


Figure 2-3. The extent of the local model domain for SFR version 0.0 together with the local deformation zones. North is in the Y-direction.

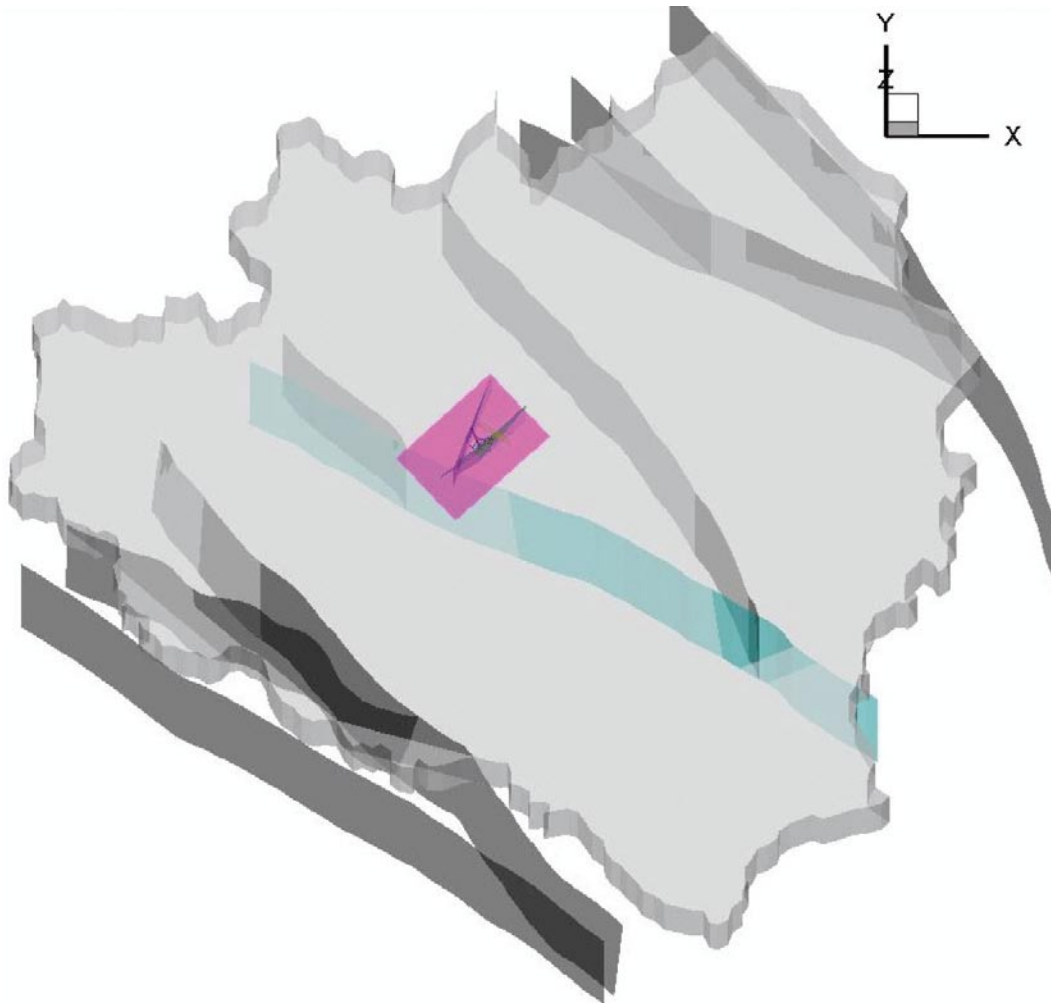


Figure 2-4. Model domain and the regional fracture zones together with the local fracture zones and the repository. North is in the Y-direction.

On the regional scale deformation zones larger than 10 km are incorporated from the Site Descriptive Model (SDM) for Forsmark v.2.2 /Stephens et al. 2007/. This is not the same data set as used in /Holmén and Stigsson 2001/. Nevertheless, it was decided to use the more recent data in the SFR0.0, as the understanding and characterization of regional zones has improved since the model in /Holmén and Stigsson 2001/. A total of nine regional zones were included from Forsmark SDM-Site. However, as the model domain was chosen to follow surface water divides, one of the zones is located outside the model domain and hence not important for the model. The regional deformation zones used in the model are listed in Table 2-1.

Table 2-1. Regional deformation zones included in the model.

Fracture zone
ZFMNW0002
ZFMNW0003
ZFMNW0806
ZFMNW0854
ZFMNW1173
ZFMWNW0001
ZFMWNW0004
ZFMWNW0036
ZFMWNW0853

The geological structures within the local domain are referred to as local fracture zones and they are identical to those used in /Holmén and Stigsson 2001/. The local fracture zones and the layout of the repository are given in Figure 2-5. The same colors as in /Holmén and Stigsson 2001/ are used to be able to better compare the two models.

2.2.3 Grid

DarcyTools employs an unstructured computational grid, which allows refinement for features of particular interest, such as tunnel walls, deformation zones and ground surface. Outside the repository region, i.e. local volume version 0.0, a maximum grid size of 128 meters is used in all directions. Inside the repository region, a maximum grid size of 32 meters is used. A finer vertical resolution near the top boundary of 2 meters is used over the whole domain. The maximum grid size at all tunnel walls is set to 2 meters. This is a more refined grid than used in /Holmén and Stigsson 2001/. In Figure 2-6 the grid representing the tunnel system is shown together with the local fracture zones.

2.2.4 Hydraulic parameters

The hydraulic properties on the regional scale are the same as the ones used for Case 2 in /Holmén and Stigsson 2001/. That is, the regional fracture zones will have a conductivity of $1.0E-5$ m/s and a hydraulic width of 50 meters, the rock mass in between will be treated as homogeneous with an effective hydraulic conductivity of $1.5E-8$ m/s, for a maximum grid size of 128 meters.

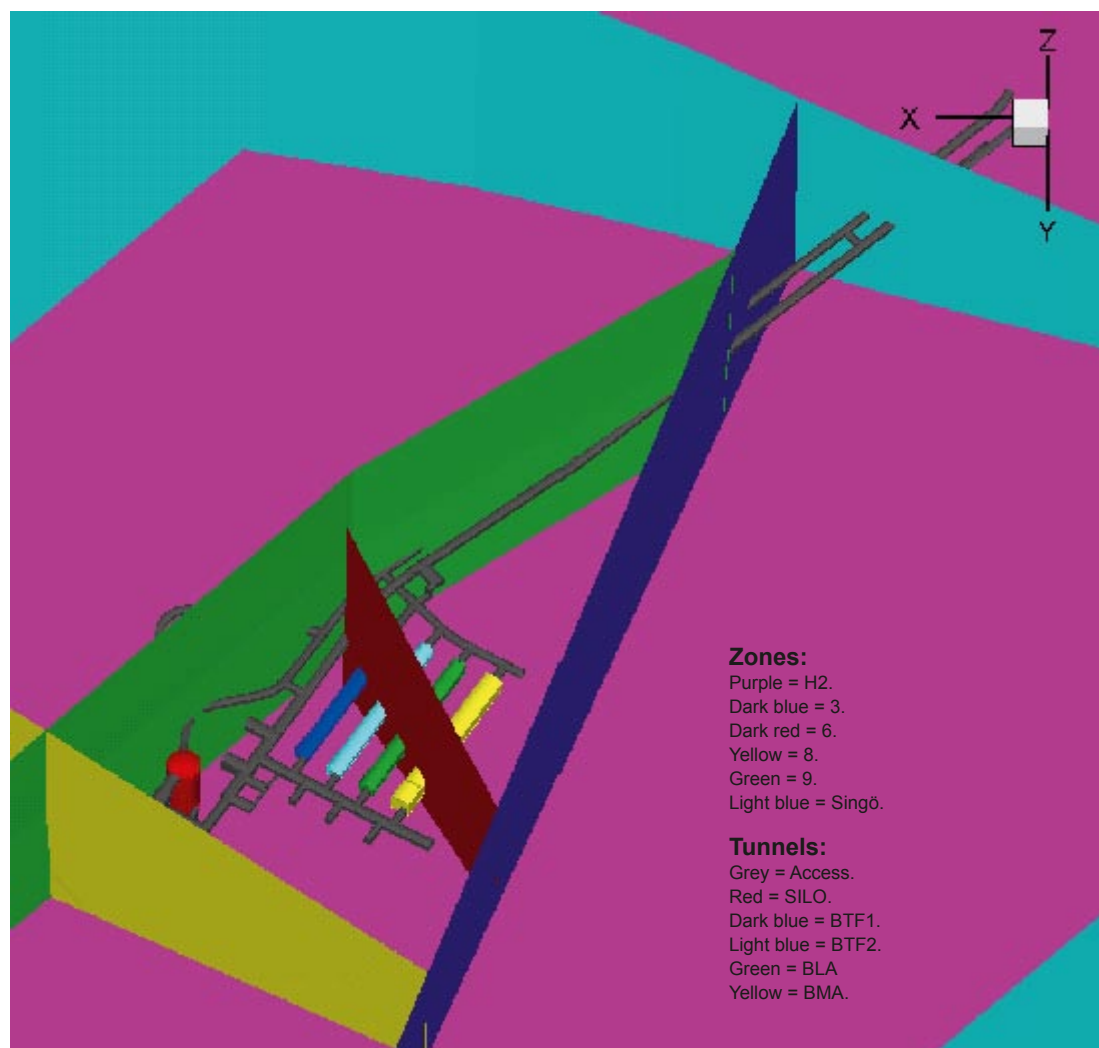


Figure 2-5. Close up of the local fracture zones for SFR version 0.0, and the layout of the tunnel system at SFR. North is in the Y-direction.

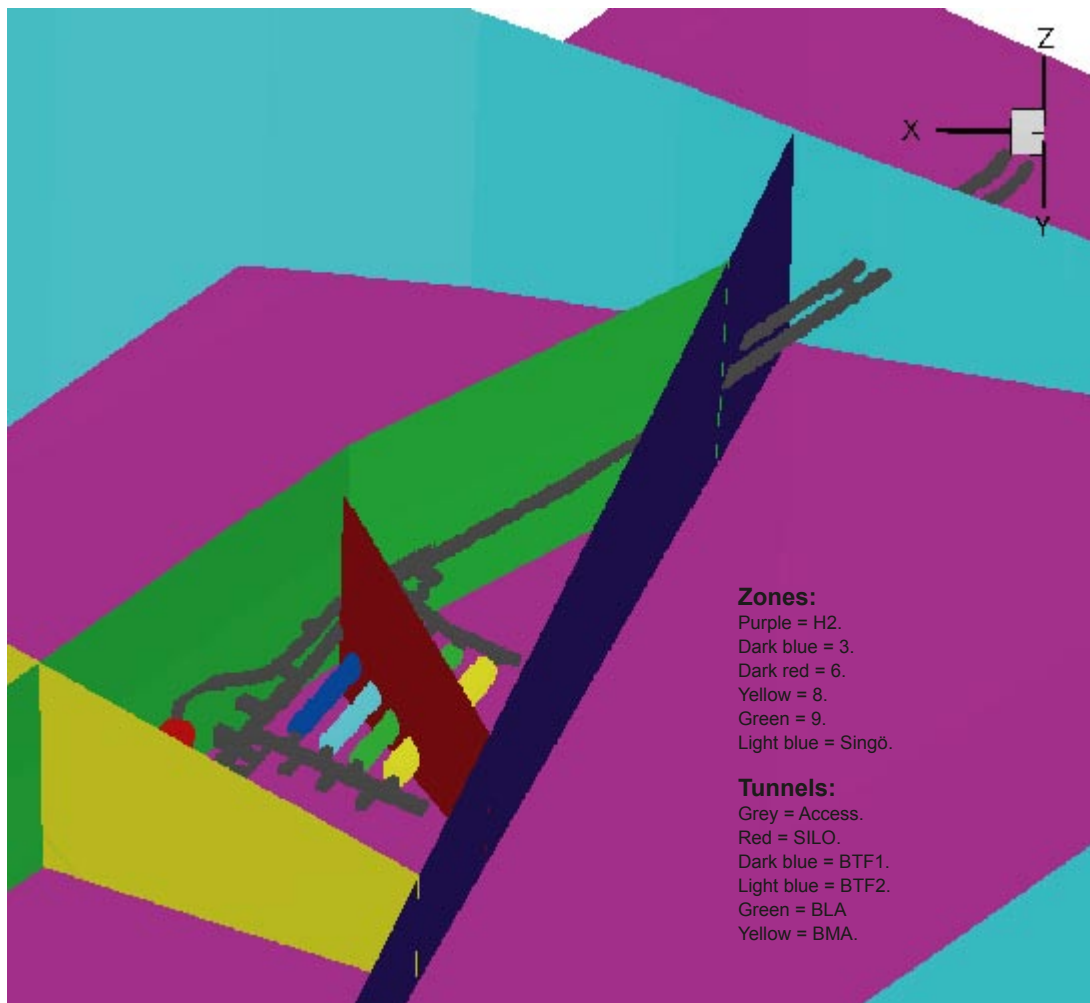


Figure 2-6. The fracture zones for SFR version 0.0, and the layout of the tunnel system at SFR as defined in the model for the calibration. That is, the computational mesh (discretisation of Figure 2-5). North is in the Y-direction.

In the first model setup (Base case) the local scale hydraulic properties, i.e. the deformation zones and rock mass inside the local scale model domain, are assigned the calibrated K-values given by Table 6.3 in /Holmén and Stigsson 2001/. Reduced conductivity (skin/grouting) and effective porosities were also taken from /Holmén and Stigsson 2001/ (see Table 6.3 and 6.5 therein). The values used are summarized in Table 2-2 and Table 2-3.

In the predictive simulations (see Sections 4 and 5) the calibrated values of the DarcyTools model will be used and low permeable tunnel plugs will be installed at roughly the same location and the same properties as in /Holmén and Stigsson 2001/. The skin is excluded in the predictive simulations, i.e. the skin/grouting is assumed to have negligible effect in the long run with saturated tunnels.

Table 2-2. Local scale hydraulic properties as defined for the first model setup.

Studied domain	Hydraulic width (m)	Conductivity (m/s)	Effective porosity (-)
Rock mass	–	6.50E-9	0.005
Zone Singö	50	1.00E-5	0.05
Zone H2	10.6	1.42E-7	0.025
Zone 3	6.45	3.18E-6	0.05
Zone 6	1.65	1.20E-6	0.025
Zone 8	10.5	3.45E-7	0.01
Zone 9	2.35	8.90E-9	0.025

Table 2-3. Grouting/Skin for different zones.

Grouting/Skin between:	Conductivity (m/s)
Access tunnel and Zone Singö	6.00E-9
Access tunnel and Zone 3	4.77E-8
BMA tunnel and Zone 6	1.20E-8
SIL0 and rock mass	1.00E-9

2.2.5 Boundary conditions

Top surface: The ground surface above sea level was assigned a net precipitation of 150 mm/year /Johansson 2008/. The computational cells below sea level are assigned prescribed head equal to hydrostatic pressure. The algorithm for describing the recharge differs between the two models; therefore the exact values from /Holmén and Stigsson 2001/ can not be incorporated in DarcyTools.

Bottom surface: The bottom of the domain (i.e. $z = -800$ m) is tentatively modeled as a no-flow boundary, same as in /Holmén and Stigsson 2001/.

Lateral surfaces: No flow boundary (surface water divide) on all lateral sides except for the north-east boundary which had a hydrostatic pressure at all times. The water divides are taken from calculated catchments for future lakes in Forsmark.

Tunnel: Atmospheric pressure in tunnels during the operational phase.

3 Open repository

3.1 Calibration

The results from the simulations, with the parameter values listed in Tables 2-2 and 2-3, together with the measured inflows from 1997 /Axelsson 1997/ are presented in Table 3-1. As can be seen the DarcyTools model with the Base case parameter values give somewhat less total inflow than the GEOAN model and the measured values for 1997. Especially the simulated inflow to the entrance tunnels is lower than the measured inflow indicating that the skin/grouting efficiency is too high or the conductivity of the Singö zone is too low. For the BMA tunnel on the other hand, the simulated inflow is higher than the measured inflow indicating that the skin/grouting efficiency is too low or the conductivity of the zone 6 is too high.

As a first step it was tested if the tunnel inflows in the GEOAN model could be repeated with the DarcyTools model by just changing the skin/grouting efficiencies and leaving the parameter values of the hydraulic structures unchanged. The inflows for one of the cases tested are presented in Table 3-2. For this case two of the skin values from Table 2-3 have been changed. These parameter values are fitted by manual calibration, i.e. by trial and error.

From Table 3-1 it can be seen that measured inflows at 1997 could be fairly match by just changing the skin efficiencies of two structures. As the objective of the calibration was to analyze if the inflows for the GEOAN model could be repeated with the DarcyTools model no further calibration was deemed needed. However, one should notice that this also tells us something about the uncertainty in the hydro model, i.e. small changes in transmissivity values for deformations zones and skin efficiency for tunnel walls could result in rather large changes in inflows to tunnels.

In conclusion, the small differences between the two models and the measured inflows were not scrutinized further and the values of the hydraulic structures according to Table 2-2 were chosen for the predictive simulations.

Table 3-1. Tunnel inflow (L/min), the table shows measured values in 1997 together with modeled values for /Holmén and Stigsson 2001/ and this work when the same parameter values are used, i.e. Base case.

Tunnel section	Measured, 1997	Model, H & S	Model, This work
Entrance tunnels	375	363	226.2
SILO	1.6	1.7	2.0
BMA	9.3	10.7	16.4
BLA, BTF and surrounding tunnels	83.6	83.3	74.2
Total	469.5	458.7	318.8

Table 3-2. Tunnel inflow (L/min) with DarcyTools for a different combination of skin/grouting, i.e. "Access tunnel and Zone Singö" = 3.0E-8 m/s and "BMA tunnel and Zone 6" = 2.0E-9 m/s. H & S inflows are shown for comparison.

Tunnel section	Model, H & S	Calibrated Model, This work
Entrance tunnels	363	357.0
SILO	1.7	2.0
BMA	10.7	10.0
BLA, BTF and surrounding tunnels	83.3	77.0
Total	458.7	446.0

4 Prediction of flow in tunnels

When defining parameter values in DarcyTools for grid cells inside an object the algorithm needs a closed “watertight” object. As the layout of the repository only was available in the form of old CAD-files it was not possible to construct solid “watertight” tunnel files. Therefore a new coarse layout of the tunnel system was constructed. These new CAD-files lacked the connection between the access tunnels and the deposition tunnels. However, as tunnel plugs should be installed between the access tunnels and the deposition tunnels the layout presented in Figure 4-1 was considered accurate enough for the predictive simulations.

Total tunnel flow is evaluated for tunnel sections at different times. The total flow in a tunnel follows definition in /Holmén and Stigsson 2001/. That is, a mass balance is taken over the tunnel section and all flows into the tunnel are summarized. The results from /Holmén and Stigsson 2001/ are summarized in Table 4-1 and the results from DarcyTools in Table 4-2.

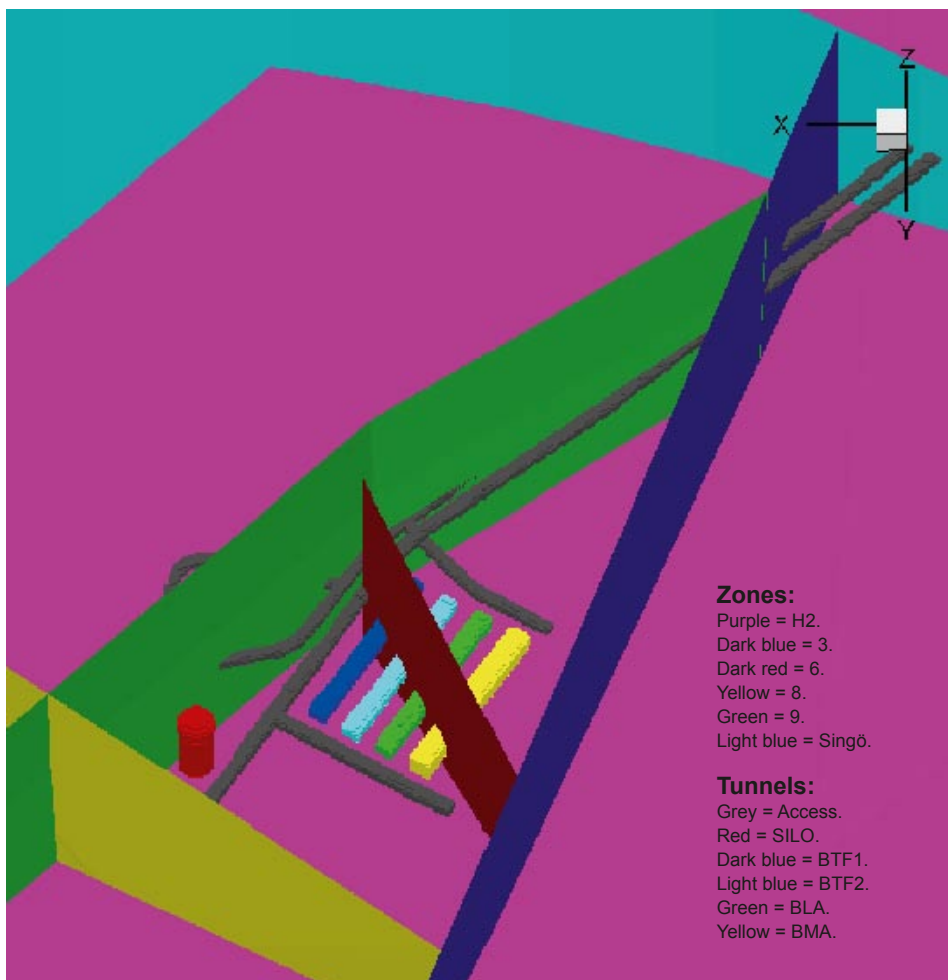


Figure 4-1. The fracture zones for SFR version 0.0, and the layout of the tunnel system at SFR as defined in the model for the predictive simulations. North is in the Y-direction.

Table 4-1. Total flow in /Holmén and Stigsson 2001/ (m³/year), Case 4, at 2000, 3000, 4000 and 5000 AD during steady state conditions.

Tunnel section	2000 AD	3000 AD	4000 AD	5000 AD
BTF1	13	38	41	43
BTF2	12	33	38	41
BLA	15	42	61	61
BMA	4.8	50	65	65
SILO	0.6	2.3	4.1	3.9
Total	45.4	165.3	209.1	213.9

Table 4-2. Total flow in DarcyTools (m³/year) at 2000, 3000, 4000 and 5000 AD during steady state conditions.

Tunnel section	2000 AD	3000 AD	4000 AD	5000 AD
BTF1	0.61	6.0	73.8	142.5
BTF2	0.60	5.8	74.5	139.1
BLA	0.71	7.1	98.8	175.0
BMA	1.16	11.6	185.2	321.7
SILO	0.13	0.56	9.2	15.8
Total	3.2	31.1	441.5	794.1

The fact that slightly different DEMs (Digital Elevation Models) are used for the two models is a possible explanation for the discrepancies observed in calculated flow, see Table 4-1 and 4-2. The flows are small and differences in topography could result in a slightly altered local flow field. By visual inspection, one can, for example, observe that some islands east and north-east of the repository are missing in /Holmén and Stigsson 2001/. Furthermore, in DarcyTools, the topography is represented by a computational mesh, which is only resolved by 2 meters in elevation. The head gradients are small under the sea; thus, it is not surprising that even small topographical discrepancies above the SFR repository influence flow predictions for 2000 AD. Another possible cause for the discrepancies relates to the orientation of the computational grid. The grid in /Holmén and Stigsson 2001/ was rotated parallel to the orientation of tunnels, whereas the SFR v.0.0 uses a grid defined by RT90 (parallel to the geographic North, respectively, East). A consequence of this grid orientation is that flow along a tunnel wall may enter and exit the tunnel along its way, and thus be artificially “counted multiple times”, i.e. an artifact owing to discretisation.

However, the most significant explanation for the discrepancies observed is the fact that /Holmén and Stigsson 2001/ aimed to match the measured excess head in bore holes from falling head tests before the repository was built. This could only be accomplished by using a time step somewhat larger than the numerically optimized in order to force the model into a transient behavior. An effect of this is a higher flow through the tunnels, and this is disturbing the flows even at 3000 AD (personal communication with Johan Holmén). Also, as different algorithms are used to calculate the actual recharge, i.e. top boundary condition, in GEOAN and DarcyTools, there may be some differences in the total water flow through the model domain.

The total flows after 2000 AD are larger but of the same order of magnitude as the one reported in /Holmén and Stigsson 2001/. However, if one looks at the flows reported from the sensitivity study in /Holmen 2005/, it is clear that the flows are within the uncertainty bounds. It should be noted that in DarcyTools simulations after 4000 AD do not reach steady state; the flows are still increasing at 5000 AD. This could be an artifact of the model domain chosen and should be further addressed with model version 0.1. Therefore no more work was done at this stage to address the issue.

5 Prediction of flow paths

In DarcyTools the particle tracking routine has two modes of operation. One is the traditional way with the particle moving along the local velocity vector, while the second method uses the so called “cell-jump” approach. Although the second approach may be more accurate for fractured media, the traditional way to illustrate the flow paths is used here in order to facilitate a comparison to the method used by /Holmén and Stigsson 2001/. However, in /Holmén and Stigsson 2001/ the particles are released at the tunnel walls in proportion to the flow. In this study the particles are released in a uniform pattern inside the tunnels, i.e. one particle is released in each tunnel grid cell. The particles will therefore travel various distances inside the tunnels before entering the bedrock. A total of 26,400 particles are released uniformly in the tunnels.

Flow paths from the repository are calculated for the stationary flow fields at 2000, 3000 and 5000 AD. During this time period the land rise relative to the sea level will exceed 15 m /Påsse 1996/; this is modeled by lowering of the sea level, similar to /Holmén and Stigsson 2001/. Flow paths at different times are visualized for 1,000 of the 26,400 particles together with the layout of the tunnel system and some of the fracture zones (Figure 5-1 to Figure 5-5).

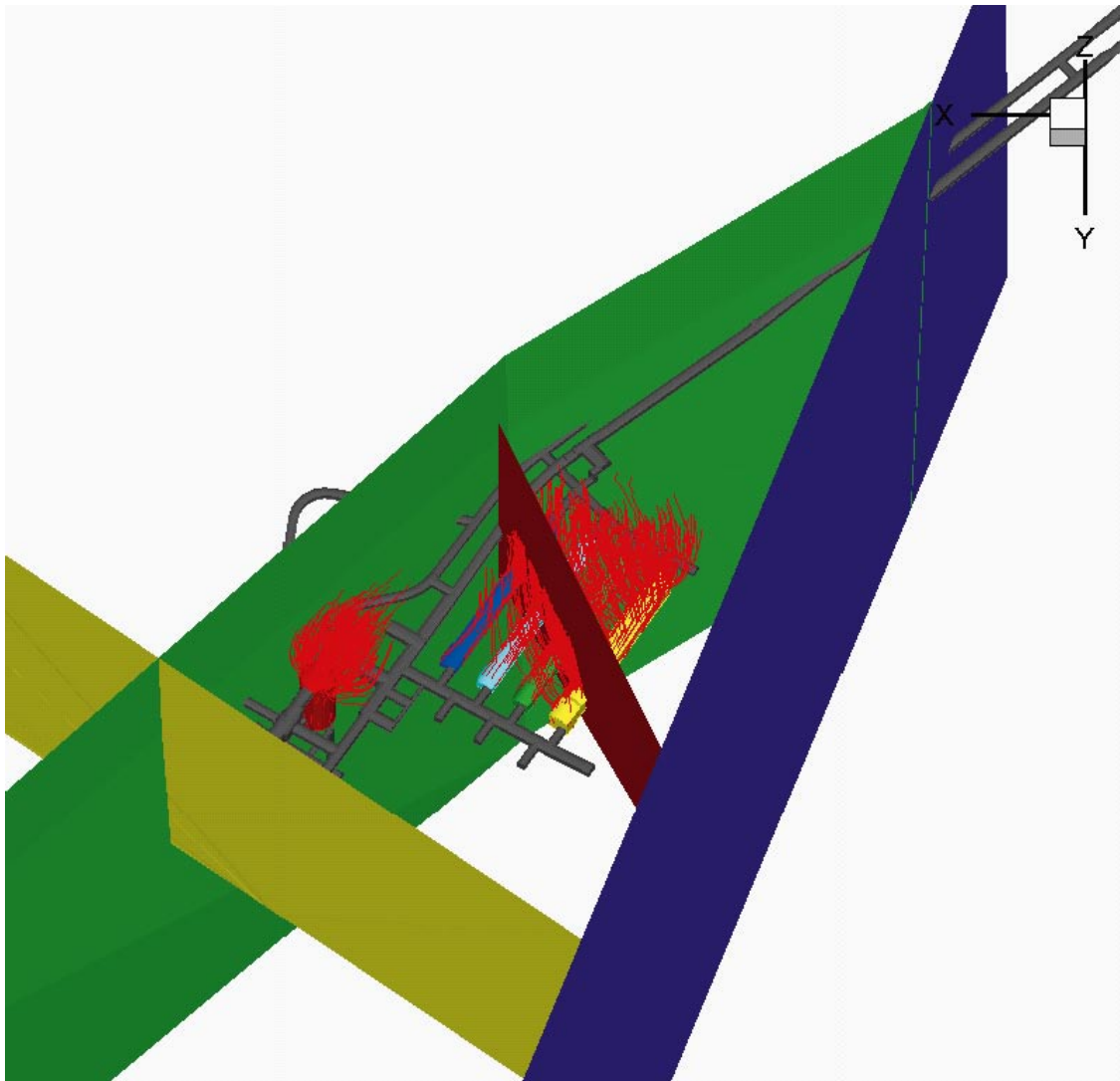


Figure 5-1. Flow paths from the SFR repository at 2000 AD. North is in the Y-direction.

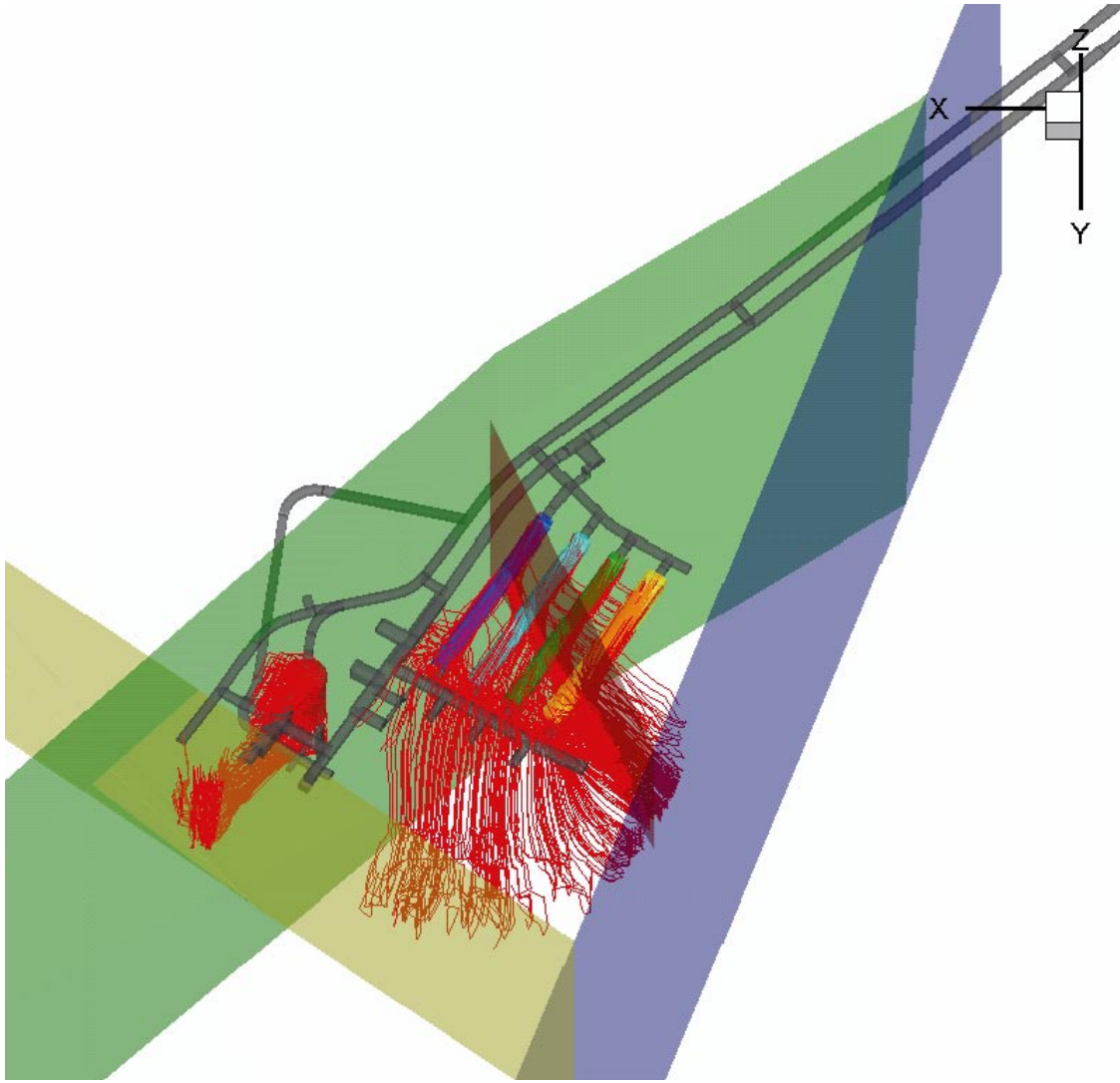


Figure 5-2. Flow paths from the SFR repository at 3000 AD. North is in the Y-direction.

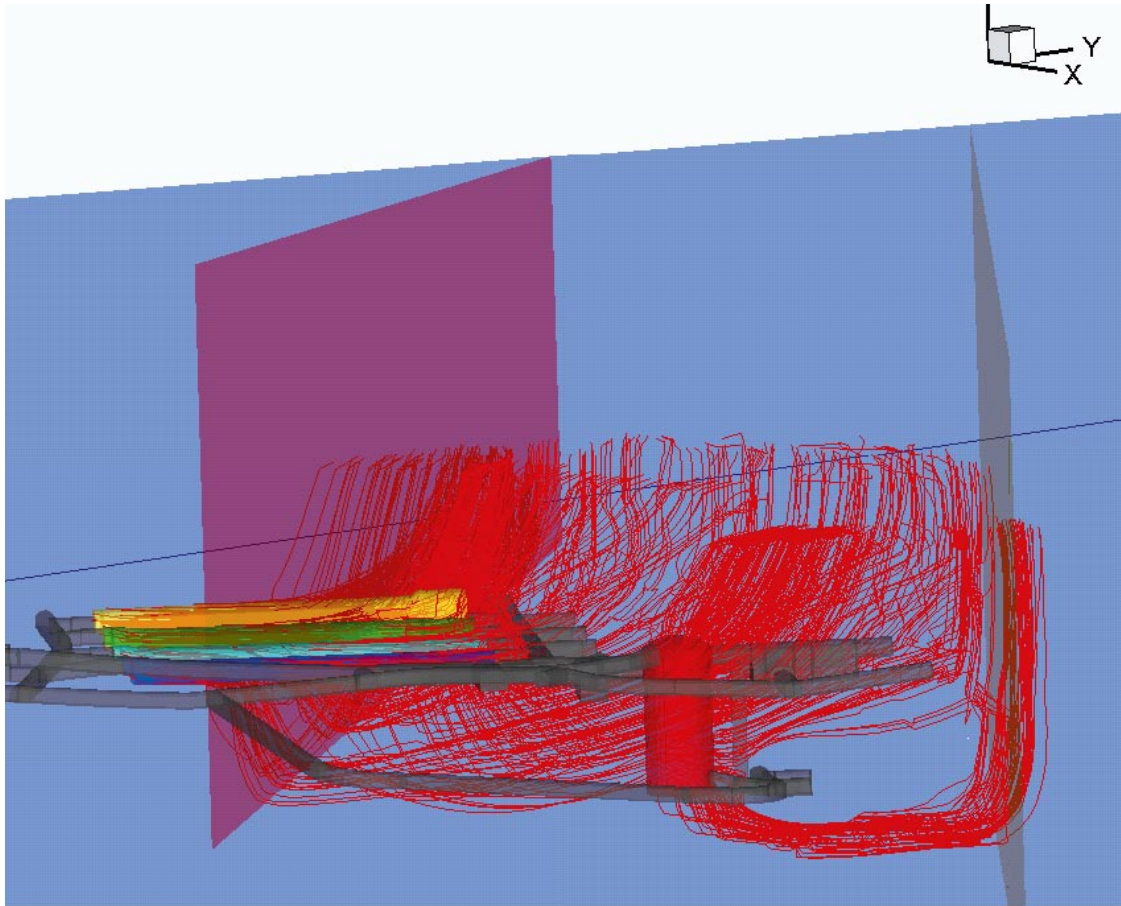


Figure 5-3. A different angle for the flow paths from the SFR repository at 3000 AD. North is in the Y-direction.

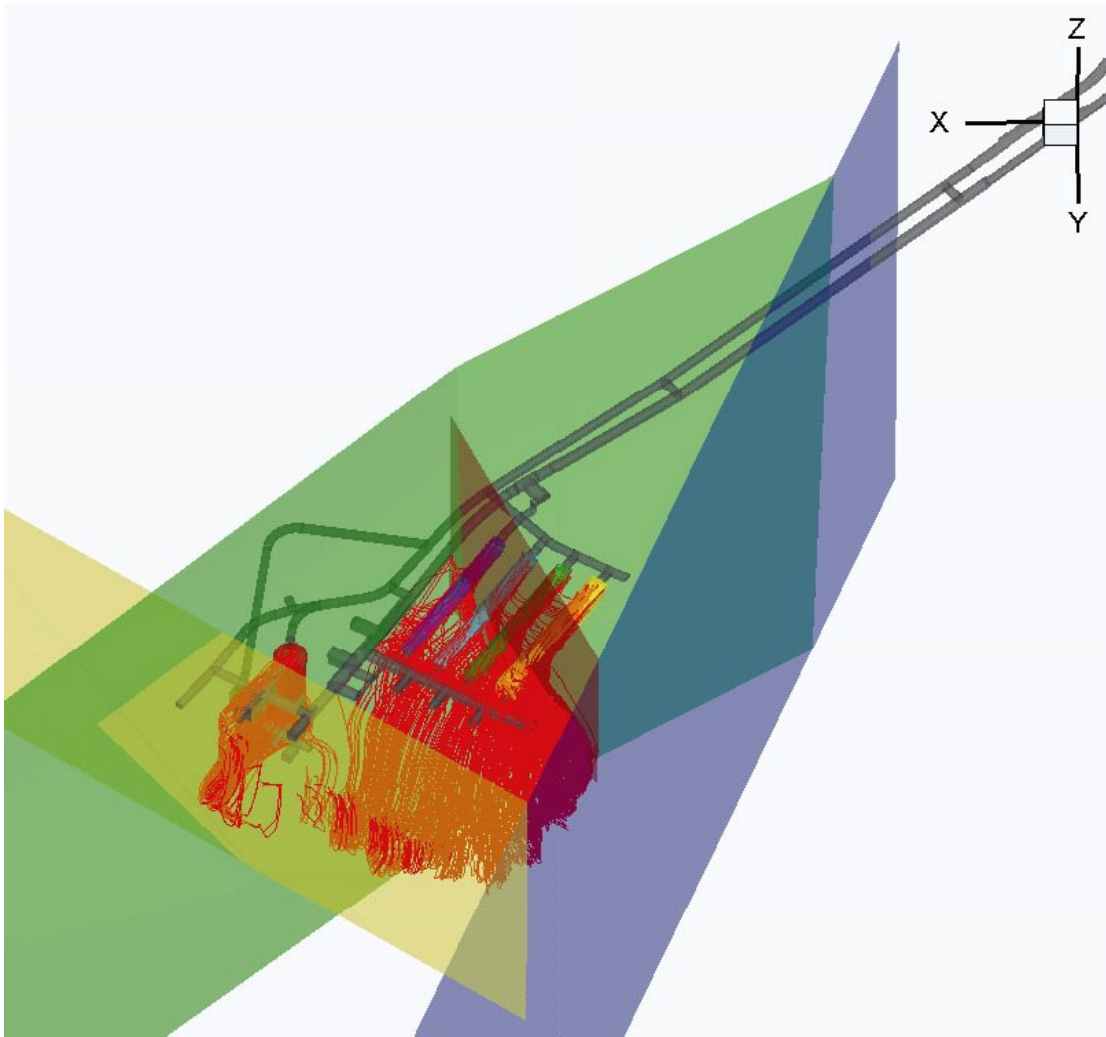


Figure 5-4. Flow paths from the SFR repository at 5000 AD. North is in the Y-direction.

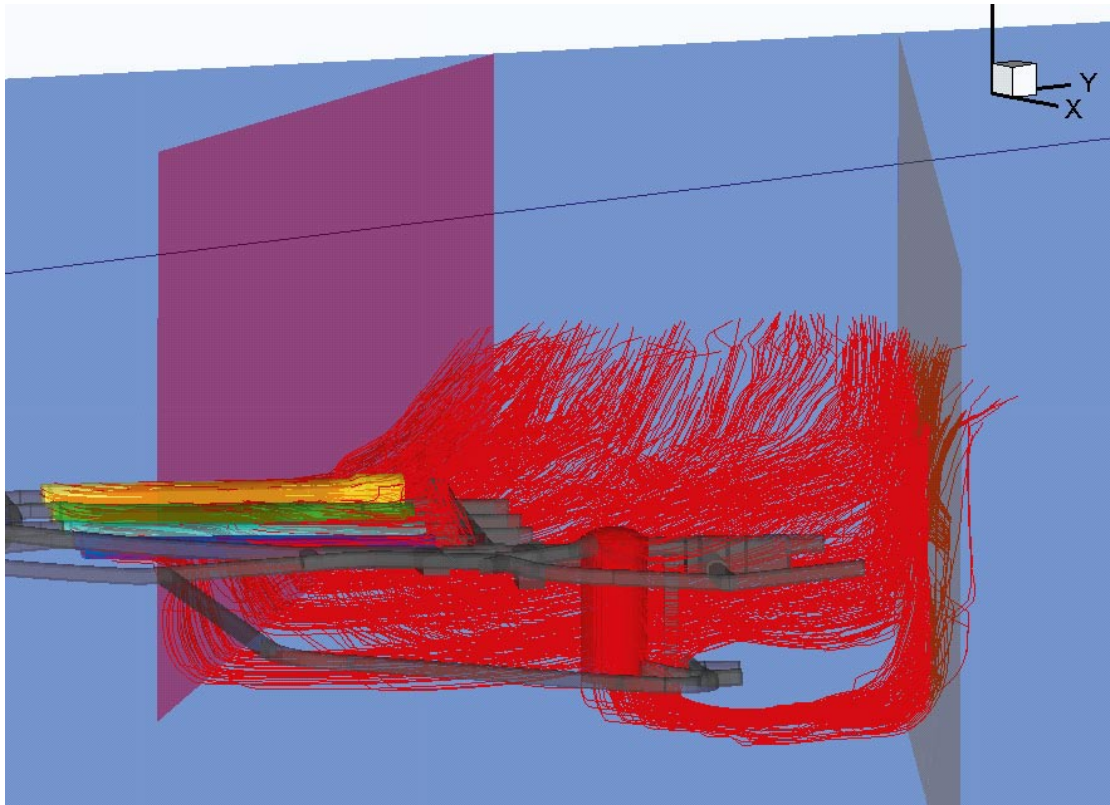


Figure 5-5. Flow paths from the SFR repository at 5000 AD. North is in the Y-direction.

Generally the flow paths develop in the same way as in /Holmén and Stigsson 2001/. That is, as long as the SFR repository is located below the sea (i.e. at 2000 AD), the flow paths are short and nearly vertical (Figure 5-1). When the shoreline is retreating, the flow field is changing markedly, the direction of the groundwater flow changes to a more horizontal flow in direction towards NNE, resulting in an increase in paths lengths (e.g. Figure 5-2). A large number of the particles are traveling in the tunnels until reaching zone 6 and then either moving up to the surface or down to zone H2 (Figure 5-2 to Figure 5-5). There are also a number of other deep flow paths reaching zone H2, and then follow zone H2 until reaching a vertical fracture zone (8 or 3) and through them discharging at the surface. The flow paths from the SILO are either directed upward or down to zone H2 and the when H2 crosses zone 8 the particles are moving upward and discharging at the surface.

The one outstanding difference between the flow paths presented here and the ones in /Holmén and Stigsson 2001/ is that in GEOAN flow paths pass through zone H2 after 3000 AD and continue deeper down in the rock mass. In DarcyTools, however, the particles that reach down to zone H2 will follow H2 horizontally until exiting through a vertical zone. The discharge areas are hence not exactly the same in the two models.

5.1 Pathway statistics

The statistics of the flow paths is based on the total number of particles released, i.e. 26,400. Two properties have been studied, breakthrough time and length of flow paths. Both statistics are presented as in /Holmén and Stigsson 2001/ with the use of percentiles. However, as the release of particles were flow-weighted in /Holmén and Stigsson 2001/ it would be *erroneous* to perform a direct comparison of percentiles with the results from DarcyTools. Also, the results presented here for 2000 AD are not directly comparable to the results from /Holmén and Stigsson 2001/ as the excess head is not reproduced in these calculations. Nevertheless, the results from /Holmén and Stigsson 2001/ are presented here as they could be interesting for the reader.

5.1.1 Length of flow paths

The length of the flow paths are presented in Table 5-1 and the ones in /Holmén and Stigsson 2001/ in Table 5-2. When studying the results from DarcyTools one should remember that the length of the flow paths presented here are including transport in the tunnels. The results are here presented with the SILO separated from the deposition tunnels.

The results from the two models are not directly comparable. However, a few things could be observed from the results. At 2000 AD the flow paths in DarcyTools are probably somewhat longer than in GEOAN, this is mainly because of the fact that transport lengths inside the tunnels are included in DarcyTools. At 5000 AD however, the flow paths are longer in GEOAN. Studying the figures illustrating the flow paths indicate that the reason is that the flow paths in GEOAN go through zone H2 while in DarcyTools the particles reaching zone H2 enters the zone and remains there until reaching zone 8 or zone 3.

5.1.2 Breakthrough times

The breakthrough times are presented in Table 5-3 and the ones from /Holmén and Stigsson 2001/ in Table 5-4. When studying the results from DarcyTools one should remember that the length of the breakthrough times presented here are including transport in the tunnels. However, as the particles move with a greater speed inside the tunnels the effect will not be as great as when calculating the length of the flow paths. The results are here presented with the SILO separated from the deposition tunnels.

As stated before the results from the two models are not directly comparable. However, a few things could be observed. There is a big difference in breakthrough times at 2000 AD, the longer breakthrough times are directly related to the small flows at 2000 AD in DarcyTools. At 5000 AD the two models show similar breakthrough times, the moderately longer times in GEOAN are probably a consequence of the longer flow paths.

Table 5-1. Length of the flow paths at 2000 and 5000 AD in DarcyTools.

Time AD	Flow path length (m)		
	10th Percentile	50th Percentile	90th Percentile
SILO			
2000 AD	55	106	296
5000 AD	159	287	332
BTF, BLA, BMA			
2000 AD	55	87	211
5000 AD	225	341	465

Table 5-2. Length of the flow paths at 2000 and 5000 AD in GEOAN, /Holmén and Stigsson 2001/.

Time AD	Flow path length (m)		
	10th Percentile	50th Percentile	90th Percentile
SILO			
2000 AD	66	66	131
5000 AD	70	355	395
BTF, BLA, BMA			
2000 AD	73	73	76
5000 AD	275	489	616

Table 5-3. Breakthrough times at 2000 and 5000 AD in DarcyTools.

Time AD	Breakthrough times (years)		
	10th Percentile	50th Percentile	90th Percentile
SILO			
2000 AD	7,598	8,732	9,593
5000 AD	87	114	168
BTF, BLA, BMA			
2000 AD	419	7,686	9,133
5000 AD	10	107	253

Table 5-4. Breakthrough times at 2000 and 5000 in GEOAN, /Holmén and Stigsson 2001/.

Time AD	Breakthrough times (years)		
	10th Percentile	50th Percentile	90th Percentile
SILO			
2000 AD	300	313	1,056
5000 AD	45	129	172
BTF, BLA, BMA			
2000 AD	58	105	319
5000 AD	141	247	497

6 Discussion

In the task description it was stated that also transient simulation should, if possible, be carried out. However, transient simulations were found too computationally demanding to reach convergence for the small flows surrounding the repository on each time step. This made the simulations practically impossible to run. One reason could be the huge difference in the flows surrounding the repository and the regional flow. The difference was around 4-5 orders of magnitude. Perhaps a coarser grid resolution could be used in the local domain surrounding the repository to reduce the computational time. Another reason for the convergence problems could be the algorithm for calculating the free groundwater surface. Large amounts of surface water needs to be transported away each time step resulting in longer calculation times and more iterations to reach steady state. Possibly, an alternative description of the surface hydrology (or top boundary condition) could improve the convergence.

One of the objectives of this study was to evaluate if the SFR model by /Holmén and Stigsson 2001/, can be numerically implemented in DarcyTools and that earlier flow results from GEOAN can be reproduced. The two numerical models are set up and parameterized as similarly as possible. However, there are some important differences. First, the boundary conditions, especially the model domain and top boundary conditions differ. That is due to different algorithms/approaches for calculating the recharge and groundwater table but also because the topographical data used in DarcyTools has higher resolution. Second, the grid is more refined, i.e. smaller grid cells, in DarcyTools, which should result in more accurate simulations. Third, in /Holmén and Stigsson 2001/ different models are used at different scales, i.e. they transfer boundary conditions from a regional grid to a local grid. This was partly because of the limited computer power available at the time. In DarcyTools, however, only one computational mesh is used with a much more refined grid in the area surrounding the repository. This should also result in more accurate simulations. Forth, updated regional fracture zone data are used in the DarcyTools model, as the original dataset used in GEOAN was unavailable. This study has demonstrated a number of typical obstacles encountered in transferring a hydrogeological model from one numerical code to another. These obstacles involve tracking previous data versions and simplifications made in the numerical implementation (such as boundary conditions and the discretisation of the computational mesh), and precludes preserving the model intact in the transfer process. Nevertheless, the modeling results agree rather well, particularly for open repository conditions.

The most noticeably difference between the results from the two models is the flows at 2000 AD due to the excess head simulated in GEOAN. Another is that the path ways in GEOAN after 3000 AD go through zone H2 and deeper down in the rock mass. In DarcyTools however, the particles goes down to H2 and than flows horizontally until they reach a vertical zone. A larger inflow to saturated tunnels (or flow in tunnels) in DarcyTools is expected because the coordinate system was not rotated parallel to the tunnel directions, as was done in GEOAN. That is, a larger tunnel surface is exposed to the flowing water results in more flux in and out of the tunnel-wall cells, i.e. some of the water only reaches the border cell. An improvement to the next model version (SFR v.0.1) could be to use a rotated coordinate system and also to update the algorithm for calculating inflow/outflow to a saturated tunnel. One improvement of the algorithm could be to use only the net inflow/outflow of each grid cell, i.e. a grid cell can only contribute to either total inflow or total outflow, not both.

It would have been interesting to study simulation results at 6000 AD to examine if a steady state is reached for the flows through the tunnels. However, at the onset of this study, the objective was to simulate flow results up to 5000 AD. The model domain and boundary conditions were thus chosen so as to ensure valid for simulations up to 5000 AD (i.e. no regards were taken to study conditions beyond 5000 AD). Therefore, the algorithm for calculating the free groundwater surface in DarcyTools failed to converge when the sea level was lowered approximately 19 m. Even for 5000 AD it was noted that the boundary influenced the groundwater table; therefore, the results presented here for 5000 AD are questionable. As the next model version (SFR v.0.1) must be valid for flow simulations beyond 5000 AD; it is important to study the water divides in more detail – and if needed – revise the model domain accordingly.

7 References

- Axelsson C-L, 1997.** “Data for calibration and validation of numerical models at SFR Nuclear Waste Repository, Forsmark, Sweden”. SKB R-98-48, Svensk Kärnbränslehantering AB.
- Holmén J G, Stigsson M, 2001.** “Modelling of future hydrogeological conditions at SFR”. SKB-R-01-02, Svensk Kärnbränslehantering AB.
- Johansson P-O, 2008.** “Description of surface hydrology and near-surface hydrogeology at Forsmark. Site descriptive modelling SDM-Site Forsmark”. SKB R-08-08, Svensk Kärnbränslehantering AB.
- Påsse T, 1996.** “A mathematical model of the shore level displacement in Fennoscandia”. SKB TR 96–24, Svensk Kärnbränslehantering AB.
- Rhén I, Follin S, Hermanson J, 2003.** “Hydrological Site Descriptive Model – a strategy for its development during Site Investigations”. SKB R-03-08, Svensk Kärnbränslehantering AB.
- Stephens M B, Fox A, La Pointe P, Simeonov A, Isaksson H, Hermanson J, Öhman J, 2007.** ”Geology Forsmark. Site descriptive modelling Forsmark stage 2.2” SKB R-07-45, Svensk Kärnbränslehantering AB.
- Strömgren M Brydsten L, 2008.** ”Digital elevation models of Forsmark. Site descriptive modelling SDM-Site Forsmark”. SKB R-08-62, Svensk Kärnbränslehantering AB.
- Svensson U, Kuylenstierna H-O, Ferry M, 2008.** DarcyTools, Version 3.1. Documentation to be written during 2008.