EFFECTIVE PROPERTY DETERMINATION FOR INPUT TO A GEOSTATISTICAL MODEL OF REGIONAL GROUNDWATER FLOW: WELLENBERG T⇒K

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Abstract

This paper describes the methodology used to estimate effective hydraulic properties for input into a regional geostatistical model of groundwater flow at the Wellenberg site in Switzerland. The methodology uses a geologically-based discrete fracture network model to calculate effective hydraulic properties for 100m blocks along each borehole.

A description of the most transmissive features (Water Conducting Features or WCFs) in each borehole is used to determine local transmissivity distributions which are combined with descriptions of WCF extent, orientation and channelling to create fracture network models. WCF geometry is dependent on the class of WCF. WCF classes are defined for each type of geological structure associated with identified borehole inflows.

Local to each borehole, models are conditioned on the observed transmissivity and occurrence of WCFs. Multiple realisations are calculated for each 100m block over approximately 4000m of borehole. The results from the numerical upscaling are compared with conservative estimates of hydraulic conductivity. Results from unconditioned models are also compared to identify the consequences of conditioning and intervals of boreholes that appear to be atypical.

An inverse method is also described by which realisations of the geostatistical model can be used to condition discrete fracture network models away from the boreholes. The method can be used as a verification of the modelling approach by prediction of data at borehole locations. Applications of the models to estimation of post-closure repository performance, including cavern inflow and seal zone modelling, are illustrated.

1 Introduction

The Wellenberg site in Switzerland has been the subject of detailed geological, geophysical and hydrogeological investigations as the proposed site for the disposal of low and intermediate level radioactive waste. The most recent phase of investigations has now been completed and documented (NAGRA 1997). The aim of the investigations was to derive geological and hydrogeological parameters and understandings for prediction of radio-nuclide transport as part of a safety assessment of the planned repository. The proposed host rock for the repository is the Cretaceous Palfris formation and Tertiary Marls. The Palfris is a highly consolidated argillaceous marl with inter-bedded limestone beds (Mazurek et al. 1998). Figure 1-1 shows a geological cross-section of the site. Seven deep boreholes have been drilled at the site of which five were nominally vertical and two inclined. These boreholes have been the subject of intensive characterisation work including core logging, geophysical logging, hydraulic testing and monitoring.

One of the key hydraulic properties measured in the boreholes is local transmissivity T (m^2/s) of discrete inflow zones. The aim of the work described here is to predict the local scale hydraulic conductivity K (m/s) for input to a geostatistical model of site scale groundwater flow. The methodology for derivation of the conductivities was called "T⇒K conversion". The T⇒K calculation method is illustrated in Figure 1-2. The underlying datasets and the steps in the methodology are discussed below.

2 The Hydraulic and Geologic Datasets

As part of the hydraulic testing performed by NAGRA, long intervals of each borehole were isolated and pumped while the borehole fluid was logged using conductivity and temperature probes. It was possible to identify inflow zones from anomalies on the conductivity and temperature logs. Quantitative estimates of inflow transmissivity may also be derived under favourable conditions (Lavanchy & Marschall 1997). Packer testing of isolated intervals was then performed and the results integrated with the fluid logging to derive a final self-consistent dataset. This dataset provided a list of identified zones, estimated transmissivity with uncertainties and detection limits for each borehole. In addition data from the packer tests and borehole monitoring has been used to provide profiles of environmental pressure and groundwater chemistry. During analysis of the packer tests estimates of radius of investigation of each test were made. This was strongly dependent on interval transmissivity and for the majority of the intervals was typically small (<10m) (Lavanchy & Marschall 1997).

Figure 2-1 shows a plot of transmissivity with vertical depth below the top of marl for five of the boreholes. The other two boreholes are close to the margin of the marl and are believed not to be typical of the repository host rock (Jaquet et al. 1997). Only quantified inflow zones are shown on the plot. Other inflow zones have been identified but were of insufficient magnitude to be quantified. There is a clear dependence of transmissivity with depth, with each borehole showing a higher transmissivity interval to about 200m below the top of marl then a transition to much lower transmissivities at depths of 500m or more. This pattern dominates the observations of feature transmissivity within the host rock and is echoed by the distribution of environmental pressure and groundwater chemistry. The pressures measured within the deeper marls are substantially below hydrostatic. The possible causes of this Under-Pressure Zone are discussed in Vinard et al. (1993).

Although the dominant inflows to the boreholes occur through discrete zones, it was also necessary to determine the properties of the rock between such zones. A small number of packer tests were performed on intervals without inflow zones. The hydraulic conductivities of these tests were between 10^{-12} and 10^{-14} m/s. In addition some tests including inflow features showed conductivities of 10^{-13} m/s or less. The effective hydraulic conductivity of the background rock volume was therefore estimated to be 10^{-13} m/s or lower (Lavanchy & Marschall 1997). It is important to note that this conductivity is probably due to a network of minor discontinuities rather than matrix flow in the strict sense.

Approximately 7 km of core was taken from the deep boreholes. The core was logged for lithology, mineralogy, type and intensity of deformation, fracture frequency, orientation, mineral infill and thickness of highly fractured zones. In addition surface outcrops were mapped to derive information at scales larger than core. Following hydraulic testing and localisation of inflow zones, the core was re-examined in detail at each inflow zone. This detailed examination provided information on one or more potential flow features for each inflow. The information gathered included lithology, degree and style of deformation, porosity and flow wetted surface. A more detailed description of the geological work can be found in Mazurek (1997).

3 T⇒K Conversion Methodology

3.1 Step 1 Evaluation of relationship between geological features and inflow zones

To extrapolate hydraulic properties away from the boreholes it is important to understand the larger-scale geometry of the Water Conducting Features (WCFs).

Key questions regarding the WCFs that needed to be addressed include:
- Which geological types of feature are associated with flow?
- Are geologic properties correlated with flow (e.g. fault orientation, thickness) ?
- How heterogeneous are flow properties within each feature?
- How well connected are the flow areas within each feature and between features?

At a larger scale it is necessary to address the potential influences of lithology, structure, stress and mineralisation on such properties. Within the T⇒K modelling the dominant depth control on transmissivity (shown in Figure 2-1) was assumed to be typical of the region around each borehole. Other work (NAGRA 1997 and Marschall et al. 1997) has considered the processes that may have caused this depth control.

Integration of core data with the observed inflow zones identified in the boreholes showed that inflow zones were associated with four types of features in the host rock:

- Class 1 Faults (cataclastic zones) in the argillaceous marl
- Class 2 Thin discrete shear zones
- Class 3 Fractured limestone boudins (either isolated or in larger structures)
- Class 4 Joints and other fractures

Class 1 features (faults) were associated with the majority of inflow zones. The fault network at Wellenberg is dense and only a fraction of all faults intersected by the boreholes correlate with inflow zones. In order to understand the hydraulic properties of the host rocks, it is important to understand the basis of this heterogeneity. For example flow might be only associated with faults that had undergone recent reactivation and hence have a particular orientation. Investigation of fault properties showed no correlation between fault orientation, thickness or mineralogy with the hydraulic properties (Mazurek 1997). Thus the observed variability of faults was assumed to relate to heterogeneity within and variability between the faults rather than to separate populations of hydraulically significant faults.

3.2 Step 2 Development of Conceptual Models of the WCF system

For each of the WCF classes a model description was developed from the available information. The level of detail was a function of the importance of the feature class and the information available. The forum for model development was a series of meetings between geologists, hydrogeologists and modellers involved in the project. The data used to parameterise the models were identified and supplemented by expert judgement. In cases where expert judgement was used, ranges of values were suggested.

The most detailed descriptions were developed for the faults (WCF Class 1). Data on all faults greater than 50cm in true thickness had been routinely collected. Data for faults thicker than 10cm had been collected in two boreholes. Orientation data was available for the largest faults and it was assumed that these were typical of the fault population. Length scale was given by a multiplier of the fault thickness (Mazurek et al. 1998). The macroscopic area of each fault was assumed to consist of a) transmissive patches (channels) which relate to the quantified inflow zones; and b) less transmissive (or off-channel) patches that would either be inflows below the limit of detection or intervals with hydraulic conductivity similar to that of the background rock. The channelling fraction (the fraction of channel patches) was calculated from the observed fraction of faults that corresponded to quantified inflow zones in the boreholes. Options for describing the heterogeneity within faults were also considered (see Mazurek et al. 1998).

The transmissivity of the fault channels and of the other hydraulically significant features were described by the transmissivity trend and a local variability derived from the integrated data set. The geometric descriptions of the other WCF classes were simpler than that developed for the faults. A subset of WCF class 3 - the Interbedded Limestone Units were however modelled deterministically throughout the study because these features might be extensive across the host rock. They are however of low hydraulic significance as the limestone elements are isolated within the structure.

3.3 Step 3 Prediction of Effective Properties

Given a description of the local WCF system around each borehole the effective hydraulic conductivities were calculated for cubes of 100m side-length along the host rock section of each of the five boreholes. Two approaches for the calculation of effective hydraulic conductivity were used (Jaquet et al. 1997).

In the "arithmetic mean approach" the local arithmetic mean transmissivity (over 100m moving window) was divided by 100m (window length) at 50m intervals. This results in an estimate of conductivity similar to that suggested by Snow (1969). It corresponds to the assumption of infinite uniformly transmissive features normal to the borehole. Where features are heterogeneous or of finite size compared to the scale at which the effective properties are required, this approach will be conservative (i.e. over-estimate hydraulic conductivity). However where the transmissive features are steeply inclined to the borehole it is necessary to correct for this orientation bias using a weighting factor (Terzaghi 1965) to determine directional hydraulic conductivity. As only an isotropic conductivity was used in the regional model the arithmetic approach provides a robust procedure that is insensitive to the geological models of WCFs.

The second approach used was the "fracture network approach" where detailed numerical models of the WCF system were constructed for each borehole and the effective conductivity calculated from the numerical models. The NAPSAC discrete fracture network model (Hartley 1998) was used within this study. The fracture network models were conditioned on observed inflow zones and major faults (cataclastic zones) for each borehole. The conditioning method used was based on that described by Chiles (1987) but modified to allow partial conditioning information (e.g. feature type and depth but no orientation). The modified method used a mix of conservative estimates and random sampling of unconditioned models. The random sampling used sample lines of similar orientation to the borehole so that bias was appropriately handled.

The transmissivity of features and patches that did not intersect the borehole, were conditioned using a borehole-specific depth trend. An error function was fitted to the observed $\log_{10}$ transmissivity values. This trend gave the local geometric mean transmissivity of hydraulically significant features (T_{chan}) with depth. The residuals from each fit were assumed to describe the local variability about the trend. The residuals were approximately normally distributed with a typical variance of about 0.5. For each borehole the "unexplained" variance from the error function fit was between 5 and 40% of the total variance in $\log_{10}$ transmissivity.

The NAPSAC calculation of effective hydraulic conductivity was performed for multiple conditioned realisations for both the central case and variants of the WCF models. Mazurek et al. (1998) discuss the effects of different models of the faults. Flows were calculated in three orthogonal directions related to the layout of the regional model. The geometric mean of the three directional conductivities was used to estimate the isotropic hydraulic conductivity. The horizontal axes of the model cubes were aligned with the major strike direction. The boundary conditions used four no-flow boundaries on faces parallel to the flow direction and constant reduced pressure boundaries on the remaining faces. Conductivity tensors could have been calculated (see Hoch et al.1998), however as an isotropic conductivity was needed, the mean of three directional conductivities was sufficient.

Both the approaches consider only the effective conductivity of the WCF system. In the upper host rock this is the dominant flow system, however where WCF transmissivity is very low (or where WCF frequency declines as suggested by Mazurek et al. 1998) the background rock conductivity may become significant. The host rock effective hydraulic conductivity K_{eff} was assumed to comprise of K_{WCF} and K_{rock} where:

1) $K_{eff} = K_{rock} + K_{WCF}$

Figure 3-1 shows a cross-plot of the arithmetic and fracture network approach derived hydraulic conductivities. Typically the fracture network estimates are one half to one order of magnitude lower than those from the arithmetic mean approach. This is due to the heterogeneity and finite feature size assumed within the fracture network approach. The estimates also show less variability because flow was simulated in a 100m cube rather than being solely dependent on the individual borehole intersections.

Detailed comparison of the two estimates showed that for one borehole the fracture network approach predicted much lower hydraulic conductivities than expected. Further modelling indicated that this was not the case when unconditioned models of this borehole were considered. The effect is due to a particularly low density of the largest faults (>1m thickness). The low density of large faults in this borehole is assumed to relate to heterogeneity of the rock mass.

A question that was also considered at this point was the validity of treating the host rock as an equivalent porous medium on a given length scale. A set of models for transmissivities typical of the repository region was constructed for cube sizes from 50m to 200m side-length. The variation between realisations and cube sizes was small indicating that models were appropriate for the prediction of fluxes at such scales. The relatively small variability between realisations is due to the small variation in transmissivity at the 100m scale. This is due to the removal of the transmissivity trend and to the choice of a single off-channel transmissivity. It is likely that fault transmissivity away from channels varies between just below the detection limit and transmissivities corresponding to the background rock or even the matrix. The models probably therefore over-estimate conductivity but with reduced variability.

The predicted effective conductivities were also evaluated against other evidence from the site. Models of the hydro-mechanical response of the rock mass to glacial unloading suggested that the hydraulic conductivity of the Under Pressure Zone must be very low - at or below those predicted here (Aristorenas and Einstein 1993). Consistency with groundwater chemistry data was considered in another study (Vomvoris et al. 1997).

3.4 Step 4 K⇒T Inverse Model and Verification

The T⇒K conversion was used as an upscaling procedure for borehole data prior to geostatistical modelling. The geostatistical model (the K Model) of the hydraulic conductivity field for the site (Jaquet et al 1997) used conditional simulation to create multiple realisations. Figure 3-2 shows a cross-section through one realisation, where elements are coloured by log conductivity (m/s). The T⇒K methodology relied on borehole data to build the detailed WCF system models, so it was necessary to determine an appropriate method for prediction of the WCF system away from the boreholes. Examination of the T⇒K results suggested a simple relationship between effective conductivity and WCF transmissivity. The relationship is given by equation 2.

2) $$\log_{10} K_{eff} = \log_{10} T_{Chan} - 2.1$$

where T_{Chan} is the local geometric mean transmissivity (see step 3.3). This relationship together with the dominant transmissivity trend and lack of evidence for major spatial controls on WCF extent or density, allowed the development of the inverse K⇒T method (Figure 3-3). The K model conductivity field is used to condition WCF system models that assume typical geometric properties. The method was tested by predicting the WCF system around borehole SB3. The predicted transmissivity profile for one realisation is shown in Figure 3-4. The match to the packer test results is good. Packer tests were also simulated using a steady state flow model, the model results were slightly greater than the observed interval transmissivities.

4 Model Applications and Conclusions

The development of the T⇒K conversion was crucial for up-scaling in a realistic manner that maximised use of geological understanding. It allowed the conversion from discrete points to continuous fields which simplified geostatistical simulation. The methodology also reduced variability by averaging over an appropriate volume and accounting for the effects of borehole sampling.

Having developed the geostatistical models based on the results of the T⇒K conversion, the K⇒T method was used to extrapolate the WCF system away from the boreholes. Models of the repository zone were developed for prediction of post closure cavern inflow, transport properties and Excavation Disturbed Zone (EDZ) effects around repository seal zones. Figure 4.1 shows a realisation of the predicted WCF system around the repository zone. The model has been cutaway to show some of the planned repository caverns (shown as red cuboids). Figure 4-2 shows a detail from sample particle tracking calculations performed using the discrete fracture network model around a single cavern.

The integration of geological understanding of the host rock gained from detailed core examination and outcrop mapping with detailed hydraulic characterisation has made it possible to build models of the WCF system that honour the observed WCF properties and are consistent with environmental pressure and groundwater chemistry data. These models are less over-conservative than previous models where only limited geological input was used to constrain WCF heterogeneity and connectivity.

The development of a combined approach using discrete fracture network models to describe variability at the 10-100m scale with a geostatistical model describing the variability at the site scale, has provided a practical framework for detailed post-closure flow modelling of a heterogeneous host rock. While not addressed in this paper, at the smaller scales required for transport modelling, detailed geological studies of feature porosity and mineralogy have been used to provide appropriate input.

References

Aristorenas GH, Einstein HH (1993) Numerical Investigation of Underpressures occurring at Wellenberg. NAGRA Internal Report, NAGRA Switzerland.

Chiles P (1987). Three dimensional geometric modelling of a fracture network. Proceedings of DOE/AECL Conference on Geostatistical, Sensitivity and Uncertainty Methods for Groundwater Flow and Radionuclide Transport Modelling. Battelle Press.

Hartley LJ (1998). NAPSAC Technical Summary Document. AEA Technology Report AEA-D&R-0271. AEAT Harwell, UK.

Hoch AR, Jackson CP, Todman S (1998) Self Consistency of a Heterogeneous Continuum Porous Medium Representation of a Fractured Medium. 3rd Äspö International Seminar

Jaquet O, Lanyon GW, Marschall P, Tauzin E (1997). The Wellenberg K-model: A geostatistical model of the host rock hydraulic conductivity. NAGRA Internal Report, NAGRA Switzerland.

Lavanchy JM, Marschall P (1997) WLB: Hydrogeological interpretation of the Wellenberg borehole data (SB1-SB6) NAGRA Internal Report, NAGRA Switzerland.

Marschall P, Vomvoris S, Jaquet O, Lanyon GW, Vinard P (1997) The Wellenberg K-model: A Geostatistical Description of Hydraulic Conductivity Distribution in the Host Rock for Site Characterisation and Performance Assessment Purposes. In proceedings of the Material Research Society Meeting Davos 1997.

Mazurek M (1997) GDSII: WLB- Geologische Eigenschaften der wasserfuhrenden Systeme. NAGRA Internal Report, NAGRA Switzerland.

Mazurek M, Lanyon GW, Vomvoris S, Gautschi A (1998). Derivation and Application of a geologic dataset for flow modelling by discrete fracture networks in low-permeability argillaceous rocks. For publication in Journal of Contaminant Hydrology.

NAGRA (1997) Geosynthese Wellenberg 1996. NAGRA Technical Report NTB 96-01, NAGRA Switzerland.

Snow DT (1969) Anisotropic permeability of porous media. Water Resources Research Volume 20(9).

Terzaghi RD (1965) Sources of error in joint surveys. Geotechnique 15, pp287-304.

Vinard P, Blumling P, McCord JP Aristorenas G (1993) Evaluation of Hydraulic Underpressures at Wellenberg, Switzerland. In Proceedings of Rock Mechanics in the 90's 34th US Symposium on Rock Mechanics, University of Wisconsin.

Vomvoris S, Pearson FJ, Waber HN, Scholtis A, Schindler M, Vinard P (1997) Consistency of hydrodynamic modelling and hydrochemical data. NAGRA Internal Report, NAGRA Switzerland.

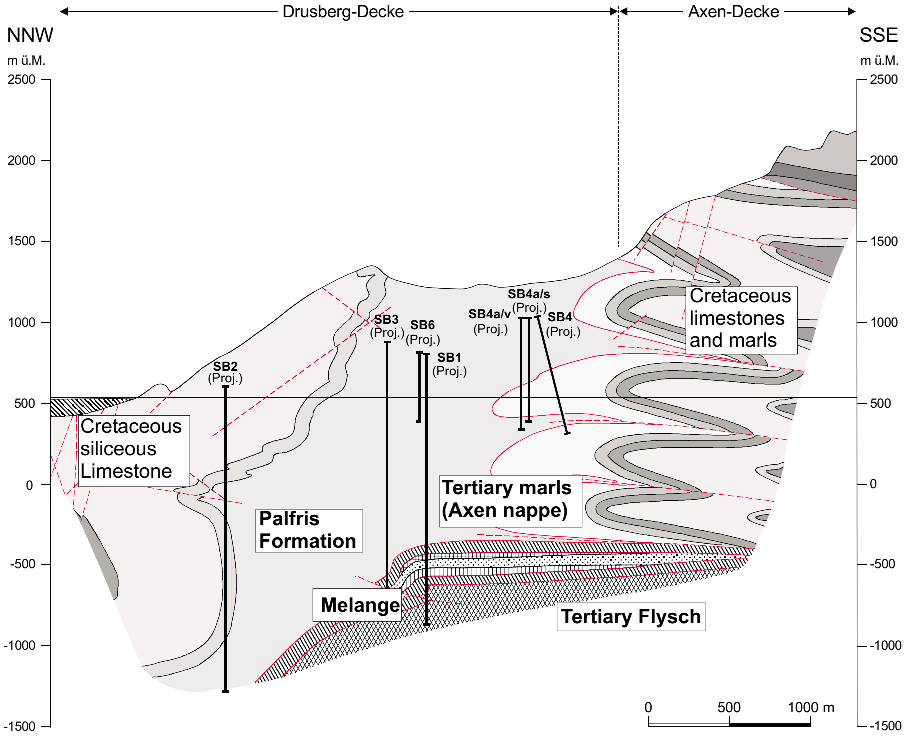

Figure 1-1 Geological section of the Wellenberg area. Borehole positions are projected onto the plane of the section.

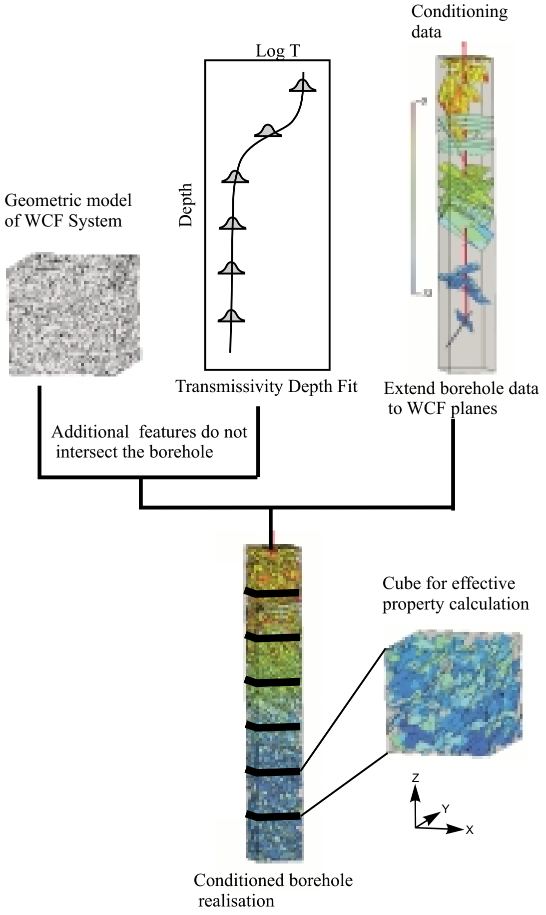

Figure 1-2 T=>K Schematic. WCF system conditioned by transmissivity trend and borehole data.

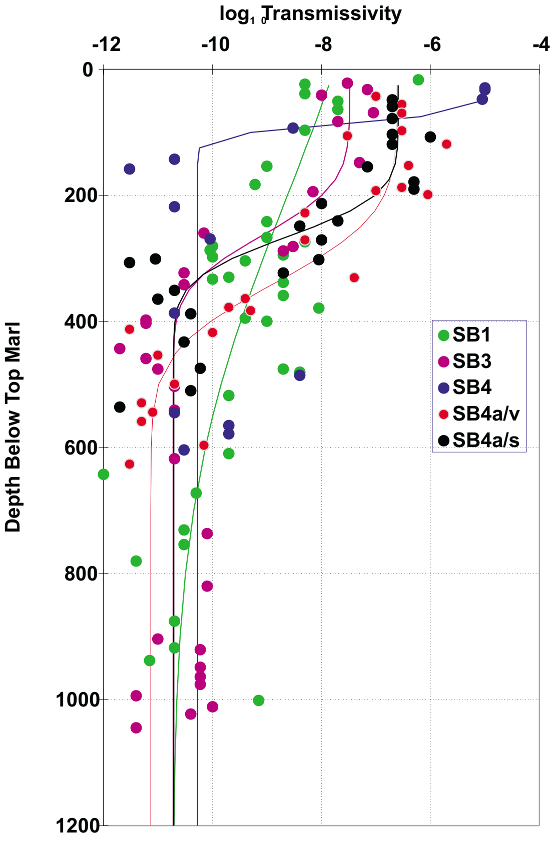

Figure 2-1 Integrated dataset inflow transmissivities for boreholes SB1,SB3,SB4,SB4a/v and SB4a/s

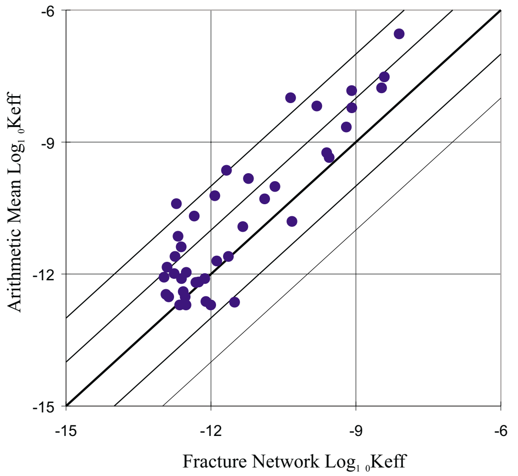

Figure 3-1 Comparison of Arithmetic Mean and Fracture Network Approach derived effective hydraulic conductivity

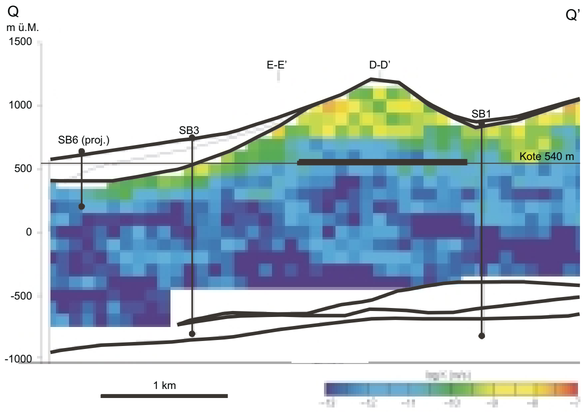

Figure 3-2 Section through sample realisation from K-Model conditional simulation using Fracture Network Approach effective conductivities.

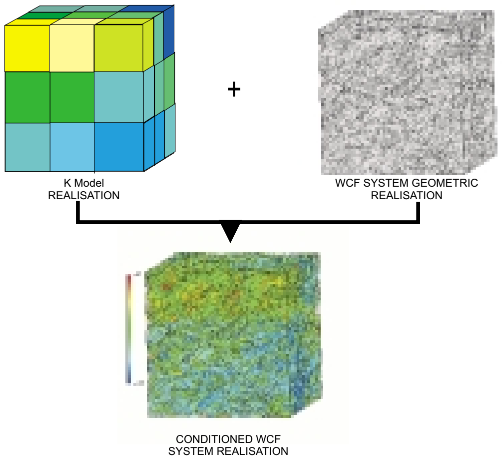

Figure 3-3 K=>T METHOD: Geometric realisations of the WCF system are conditioned on realisations of the hydraulic conductivity field from K model conditional simulations

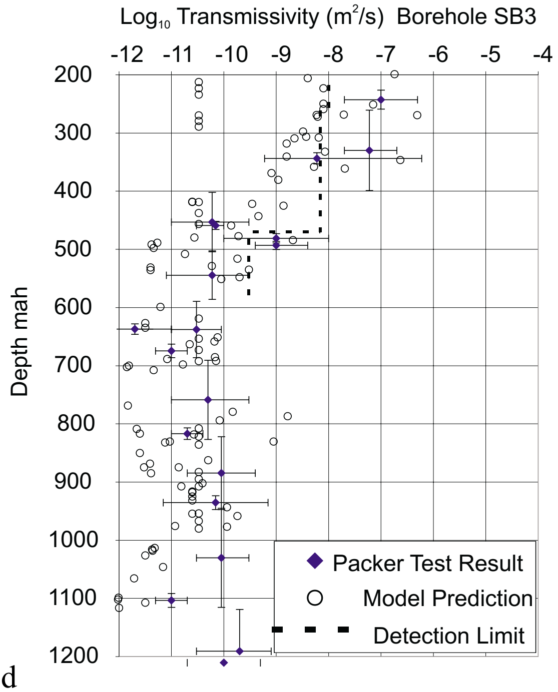

Figure 3-4 Predicted inflow transmissivities and packer test measurements for borehole SB3.

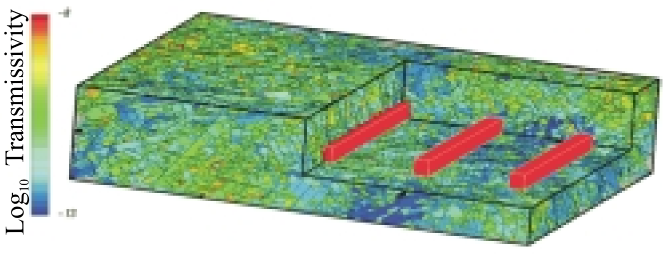

Figure 4-1 Predicted WCF system around repository caverns.

Figure 4-2 Cutaway of WCF system around a cavern and sample particle tracks.