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National Cooperative for
the Disposal of Radioactive Waste

TECHNICAL REPORT 91-03

GRIMSEL TEST SITE

MODELING OF GROUNDWATER FLOW IN THE ROCK BODY SURROUNDING THE UNDERGROUND LABORATORY

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A JOINT RESEARCH PROGRAM BY

- NAGRA – National Cooperative for the Storage of Radioactive Waste, Wettingen, Switzerland
- BGR – Federal Institute for Geoscience and Natural Resources, Hannover, Federal Republic of Germany
- GSF – Research Centre for Environmental Sciences, Munich, Federal Republic of Germany

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FOREWORD

Concepts for the disposal of radioactive waste in geological formations lay great weight on acquiring extensive knowledge of the proposed host rock and the surrounding rock strata. For this reason, Nagra has, since May 1984, been operating the **Grimsel Test Site (GTS)** which is located at a depth of 450 m in the crystalline rock of the Aare Massif of the Central Swiss Alps. The general objectives of the research being carried out in this underground laboratory include

- the build-up of know-how in planning, performing and interpreting field experiments in various scientific and technical disciplines and

- the acquisition of practical experience in the development of investigation methodologies, measuring techniques and test equipment which will be of use during actual repository site explorations.

The GTS is operated by Nagra and, on the basis of a German-Swiss co-operative agreement, various experiments are carried out by Nagra, the "Bundesanstalt für Geowissenschaften und Rohstoffe, Hannover" (BGR) and the "Forschungszentrum für Umwelt und Gesundheit, München" (GSF). The Grimsel projects of both GSF and BGR are supported by the German Federal Ministry for Research and Technology (BMFT). NTB 85-46 (German version NTB 85-47) provide an overview of the German-Swiss investigation programme. In a special issue of the Nagra Bulletin 1988 (German version "Nagra Informiert 1+2/1988") the status of the programme up to 1988 is described.

VORWORT

Bei Konzepten, welche die Endlagerung radioaktiver Abfälle in geologischen Formationen vorsehen, ist die Kenntnis des Wirtgesteins und der angrenzenden Gesteinsschichten von grundlegender Bedeutung. Die Nagra betreibt deshalb seit Mai 1984 das **Felslabor Grimsel (FLG)** in 450 m Tiefe im Kristallin des Aarmassivs. Die generelle Zielsetzung für die Arbeiten in diesem System von Versuchsstollen umfasst insbesondere

- den Aufbau von Know-how in der Planung, Ausführung und Interpretation von Untergrundversuchen in verschiedenen wissenschaftlichen und technischen Fachgebieten, und

- den Erwerb praktischer Erfahrung in der Entwicklung und der Anwendung von Untersuchungsmethoden, Messverfahren und Messgeräten, die für die Erkundung von potentiellen Endlagerstandorten in Frage kommen.

Im Felslabor der Nagra werden, auf der Basis eines deutsch-schweizerischen Zusammenarbeitsvertrages, verschiedene Versuche von den beiden deutschen Partnern Bundesanstalt für Geowissenschaften und Rohstoffe, Hannover (BGR) und Forschungszentrum für Umwelt und Gesundheit GmbH, München (GSF) durchgeführt. Das Deutsche Bundesministerium für Forschung und Technologie (BMFT) fördert die Arbeiten der BGR und der GSF im FLG. Der NTB 85-47 (englische Version NTB 85-46) enhält eine Uebersicht des FLG und die Zusammenfassung der Untersuchungsprogramme mit Status August 1985. In der Ausgabe 1+2/1988 des Heftes "Nagra informiert" bzw. der englischen Spezialausgabe "Nagra Bulletin 1988" ist der Stand der FLG Arbeiten anfangs 1988 beschrieben.

Der vorliegende Bericht wurde im Rahmen der erwähnten Zusammenarbeitsverträge erstellt. Die Autoren haben ihre eigenen Ansichten und Schlussfolgerungen dargelegt. Diese müssen nicht unbedingt mit denjenigen der Nagra oder des beteiligten Partner übereinstimmen.

AVANT-PROPOS

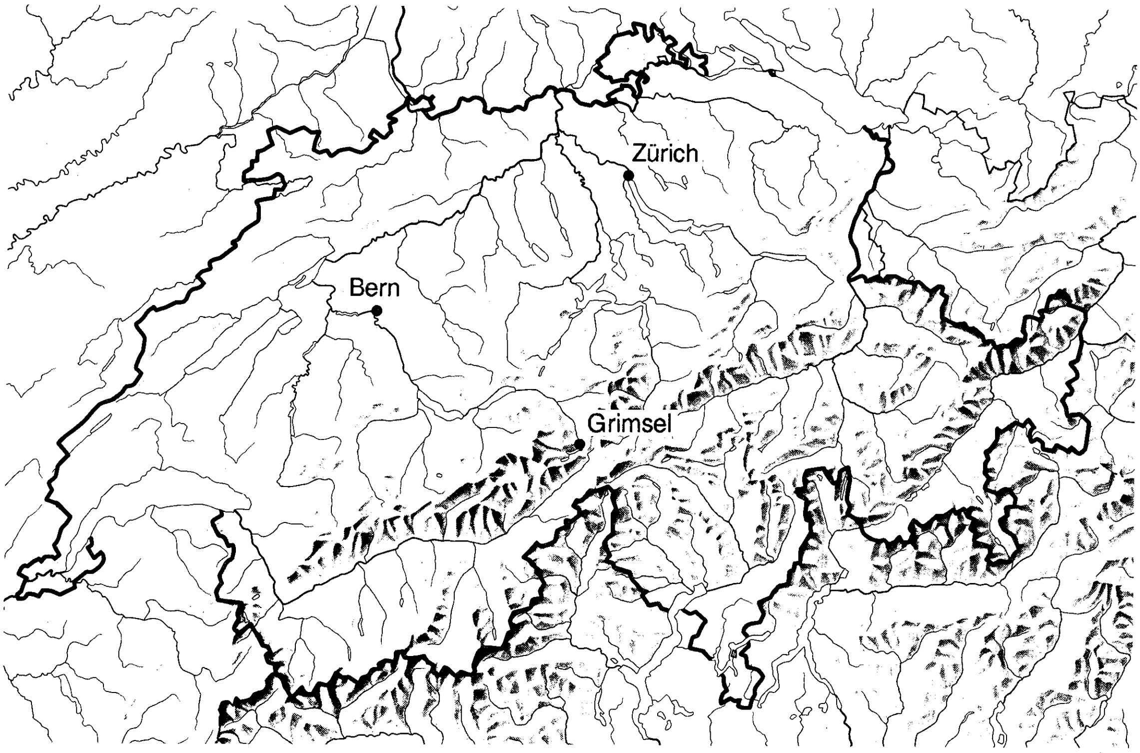
Lors d'études de concepts d'évacuation de déchets radioactifs dans des formations géologiques, on attache une grande importance à l'acquisition d'informations étendues sur la roche d'accueil et les formations rocheuses environnantes. C'est pour cette raison que la Cédra exploite depuis mai 1984 son **Laboratoire souterrain du Grimsel (LSG)** situé à 450 m de profondeur dans les roches cristallines du massif de l'Aar, situé au centre des Alpes suisses. Les principaux objectifs des recherches effectuées dans ce laboratoire concernent

- l'acquisition de savoir-faire dans diverses disciplines techniques et scientifiques pour la conception, la réalisation et l'interprétation d'expériences dans le terrain et

- la récolte d'expériences pratiques dans la mise au point de méthodologies d'investigation, de techniques de mesure et avec les appareillages qui pourraient être utilisés lors de l'exploration de sites potentiels de dépôts finals.

Le LSG est exploité par la Cédra et diverses expériences y sont réalisées par celle-ci et deux Institutions allemandes, la "Bundesanstalt für Geowissenschaften und Rohstoffe, Hannover" (BGR) et le "Forschungszentrum für Umwelt und Gesundheit GmbH, München" (GSF) dans le cadre d'un traité de collaboration germano-suisse. Les projets poursuivis au Grimsel par la BGR et le GSF sont supportés par le Ministère fédéral allemand de la recherche et de la technologie (BMFT). Les rapports NTB 85-46 (version anglaise) et NTB 85-47 (version allemande) présentent un aperçu du laboratoire souterrain et un résumé des programmes de recherches. La situation de ce programme en 1988 est présentée dans la publication "Cédra informe 1+2/1988" (version française) et "Nagra informiert 1+2/1988" (version allemande) ainsi que dans une édition spéciale en anglais (Nagra Bulletin 1988).

Le présent rapport a été élaboré dans le cadre des accords de collaboration mentionnés. Les auteurs ont présenté leurs vues et conclusions personnelles. Celles-ci ne doivent pas forcément correspondre à celles de Nagra ou ses partenaires participants.



Reproduziert mit Bewilligung des Bundesamtes für Landestopographie vom 19.6.1991

Location of Nagra's underground test facility at the Grimsel Pass in the Central Alps (Bernese Alps) of Switzerland (approximate scale 1 cm = 25 km).

Geographische Lage des Nagra Felslabors am Grimselpass (Berner Oberland) in den schweizerischen Zentralalpen (Massstab: 1 cm = ca. 25 km)

GRIMSEL-GEBIET

Blick nach Westen

1 Felslabor
2 Juchlistock
3 Räterichsbodensee
4 Grimselsee
5 Rhonetal

GRIMSEL AREA

View looking West

1 Test Site
2 Juchlistock
3 Lake Raeterichsboden
4 Lake Grimsel
5 Rhone Valley

FLG FELSLABOR GRIMSEL
GTS *GRIMSEL TEST SITE*

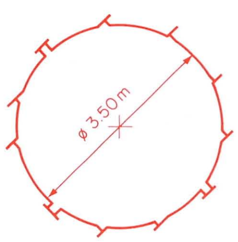
Situation

0 — 100 m

- Zugangsstollen/*Access tunnel*
- Fräsvortrieb/*by tunnel boring machine*
- Sprengvortrieb/*excavated by blasting*
- Zentraler Aaregranit ZAGR / *Central Aaregranite CAGR*
- Biotitreicher ZAGR / *CAGR with high content of biotite*
- Grimsel-Granodiorit / *Grimsel-Granodiorite*
- Scherzone/*Shear zone*
- Lamprophyr/*Lamprophyre*
- Wasserzutritt/*Water inflow*
- SB — Sondierbohrung/*Exploratory borehole*
- US — US Bohrung/*US borehole*

ZB	Zentraler Bereich/*Central facilities*
AU	Auflockerung/*Excavation effects*
BK	Bohrlochkranz/*Fracture system flow*
EM	El.magn. HF-Messungen/*-measurements*
FRI	Kluftzone/*Fracture zone investigation*
GS	Gebirgsspannungen/*Rock stresses*
HPA	Hydr. Parameter/*Hydr. parameters*
MI	Migration/*Migration*
MOD	Hydrodyn. Modellierung/*H. modeling*
NM	Neigungsmesser/*Tiltmeters*
UR	Untertageradar/*Underground radar*
US	Seismik/*Underground seismic testing*
VE	Ventilationstest/*Ventilation test*
WT	Wärmeversuch/*Heat test*

A — A Schnitt/*Section*



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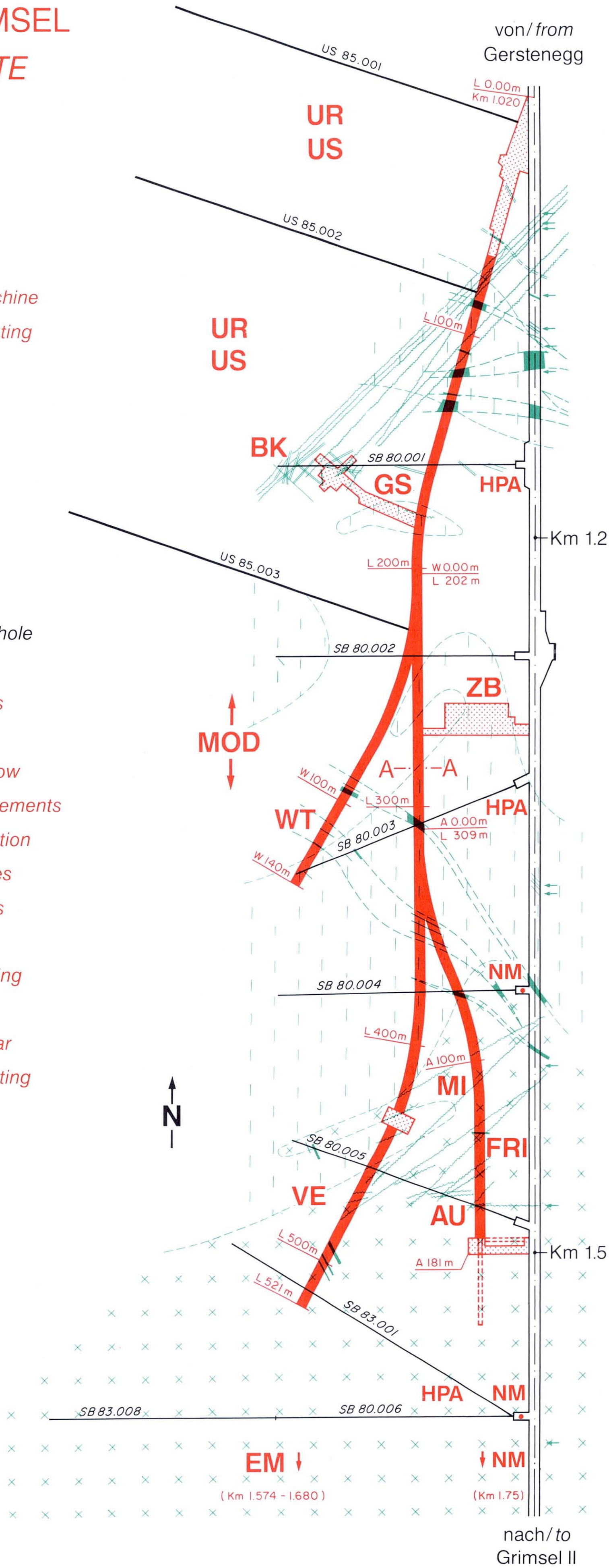

SUMMARY

One of the principal objectives of the research performed at the Grimsel Test Site (GTS) is to build-up know-how in planning, execution and interpretation of underground experiments in different scientific domains. In the scope of the hydrogeologic test program, the project MOD investigates the adequate strategy in hydrodynamic modeling of groundwater flow in a fractured rock body surrounding the GTS. The specific aims of this project were, therefore, to

- develop and test new numerical tools and techniques related to mesh generation, pre- and post-processing and to determine appropriate calibration/validation procedures and criteria
- support the interpretation of hydrologic in-situ experiments within the GTS test program and
- clarify some fundamental questions concerning the modeling of hydrodynamic effects in fractured rock around underground constructions

This report demonstrates that the adopted approach of hybrid modeling following a hierarchical model structure (different scales) is a useful method for characterization of the groundwater flow through a fractured rock massif on the regional scale (i.e. considering the large-scale anisotropy) as well as on the local scale (around underground excavation). Such modeling also provides a basis for future hydrodynamic modeling of the near-field of a rock laboratory (or repository site). The report describes the results obtained from calculations with the regional and local hydrogeologic model. A proposed calibration method is demonstrated through a simple example of the local model. The general aspects of modeling with a limited amount of data and related problems are discussed. The experience gained in project MOD shows that such modeling requires an iterative procedure with checking and updating the various model assumptions at each step.

ZUSAMMENFASSUNG

Eine der wichtigsten Zielsetzungen für die im Felslabor Grimsel (FLG) durchgeführten Arbeiten gilt dem Aufbau von Know-how in Planung, Ausführung und Auswertung von Untergrundversuchen in verschiedenen naturwissenschaftlichen Bereichen. Im Rahmen des hydrogeologischen Untersuchungsprogramms soll das Projekt MOD die geeignete Vorgehensweise bei hydrodynamischer Modellierung der Grundwasserströmung im geklüfteten Gebirge um das FLG untersuchen. Die projektbezogenen Zielsetzungen sind deshalb wie folgt ausgerichtet:

- Weiterentwicklung und Erprobung des Arbeitsinstrumentariums bezüglich Netzaufbau, Pre- und Postprocessing, sowie geeigneter Methodik für Kalibrierung/Validierung zukünftiger Standortmodelle
- Bereitstellung einer Interpretationsbasis für die im Felslabor durchgeführten hydrologischen In-situ-Versuche
- Abklärung einiger grundsätzlichen Fragen, die sich im Zusammenhang mit Modellierung der hydrodynamischen Auswirkungen von Untertagebauten im geklüftetem Gebirge ergeben

Im Bericht wird gezeigt, dass die gewählte Vorgehensweise einer hybriden und hierarchisch struktuierten Modellierung (mehrstufig mit jeweils abnehmender Skalengrösse) geeignet ist, um sowohl die regionalen (Gebirgsanisotropie) als auch die kleinräumigen (Stollenumgebung) Fliessverhältnisse im geklüfteten Fels zu charakterisieren. Der Bericht beschreibt die Resultate der Simulationen mit dem regionalen und lokalen Modell. Die als geeignet vorgeschlagene Kalibrierungsmethode wird am Beispiel des Lokalmodells veranschaulicht. Die im Hinblick auf zukünftige Standortuntersuchungen allgemein gültigen Aspekte der Grundwasser-Modellierung in Gebieten mit geringer Datendichte werden diskutiert und die sich daraus ergebenden Probleme aufgezeigt. Die im Projekt MOD gewonnene Erfahrung zeigt, dass eine solche Modellierung iterativ durchzuführen ist, mit Ueberprüfung und Anpassung der Modellannahmen nach jedem Schritt.

RESUME

L'un des objectifs principaux des recherches effectuées au laboratoire du Grimsel (GTS) est d'acquérir des connaissances dans la planification, l'exécution et l'interprétation d'expériences souterraines dans différents domaines scientifiques. Dans le cadre du programme hydrogéologique, le projet MOD a pour but d'étudier une stratégie adaptée pour la modélisation hydrodynamique des écoulements dans les roches fracturées entourant le GTS. Les buts spécifiques de ce projet sont:

- de développer et de tester des outils et des techniques numériques permettant de générer des réseaux (méthodes de "pre-" et "post-processing") et de déterminer des critères et procédures appropriés de calibration et de validation,
- d'aider à l'interprétation d'expériences hydrauliques in-situ du programme de tests GTS et
- de clarifier quelques questions fondamentales concernant la modélisation d'effets hydrodynamiques dans les roches fracturées entourant les constructions souterraines.

Ce rapport démontre que l'approche de modélisation hybride adoptée - modèles emboîtés, hiérarchisés selon les différentes échelles - est une méthode adaptée pour la caractérisation des écoulements à l'intérieur d'un massif fracturé. Cette méthode permet de caractériser les écoulements à l'échelle régionale (en considérant l'anisotropie correspondante) ainsi que ceux à l'échelle locale, à proximité des constructions souterraines. De plus, ce type de modèle servira de base aux modélisations hydrodynamiques futures qui seront réalisées à l'échelle du laboratoire ou du site d'entreposage. Le rapport décrit les résultats obtenus à l'aide du modèle hydrogéologique régional et de son équivalent local. Une méthode de calibration est proposée, dont l'application est illustrée à l'aide d'un exemple du modèle local. On discute les aspects généraux de la modélisation en présence d'un nombre de données limité, et on évoque les problèmes liés à cette question. L'expérience acquise lors du projet MOD montre qu'une telle modélisation requiert la mise en oeuvre d'un processus itératif permettant de vérifier et de modifier, lors de chaque étape, les différentes hypothèses du modèle.

GRIMSEL TEST SITE: MODELING OF THE GROUNDWATER FLOW IN THE ROCK BODY SURROUNDING THE UNDERGROUND LABORATORY

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1 INTRODUCTION

1.1 Project MOD

The task of three-dimensional modeling of groundwater flow in the jointed granitic massif surrounding the Grimsel Test Site (GTS), designated as Project MOD, was initiated by Nagra in 1988 as a part of the hydrologic investigation programme. The main objectives of the project are the following:

- To build up general experience in numerical modeling of the hydrodynamic effects around underground constructions with regards to future repository site investigations. This acquisition of know-how also involves the development and testing of new numerical tools and procedures concerning the pre- and post-processing of data, mesh generation and calibration/ validation of future repository site models.

- To provide a basis for the interpretation of the hydrogeologic GTS experiments.

- To increase the general understanding of the hydrologic behaviour of low-permeable fractured crystalline rock.

Therefore, the project MOD pursues the general investigation strategy of the GTS in the sphere of hydrodynamic modeling. The task of groundwater flow simulation in the surroundings of a rock laboratory or repository site gives rise to some fundamental questions outlined below, which should also be clarified by the modeling of the GTS:

- Given the wide-scale variation of the relevant structures (faults, joint systems, underground openings, boreholes etc.), what is the procedure to achieve an optimum discretization of the model grid?

- How feasible is a realistic assessment of the boundary conditions?

- What are the requirements and possibilities for calibration and validation of the models?

1.2 Scope of the Report

The present report describes the aim, scope and final results of the project MOD, which has been realized at several stages in the years 1988-1990. It incorporates the Internal Annual Reports (VOBORNY 1989, ADANK & VOBORNY 1990) which have provided information about work in progress and comprehensive discussion of the results. In accordance to the general nature of the GTS investigation strategy, the present report places emphasis on presentation of statements and findings of general, i.e. site-independent, importance rather than on detailed discussion of the site-specific model results.

Chapter 1 gives a presentation of the Grimsel Test Site investigation program and describes the scope and purpose of project MOD.

Chapter 2 provides an outline of the geological and hydrological setting of the project site, while the following **Chapter 3** deals with the different steps of hydrodynamic modeling.

Chapter 4 describes the data base available and corresponding evaluations for modeling purposes.

Chapters 5 and 6 present the results of the regional and local models, respectively. The calibration method proposed in Chapter 3 is demonstrated by a simple application in the local model (Chapter 6).

Chapter 7 is dedicated to the discussion of validation methodology for site-specific hydrodynamic models.

Chapter 8 presents the conclusions drawn from project MOD and recommendations for further works.

2 GEOLOGICAL OVERVIEW

2.1 Rock Structure

The Aar Massif of the Grimsel area consists of a granite and granodiorite formation of Variscan age. The granitic rock mass was locally intruded by younger dykes of acidic aplites and basic lamprophyres. In contrast with the rare aplites, the dark lamprophyre dykes occur frequently at the GTS and their contact zones with the adjacent host rock play an important role in ground water flow through the rock. All rocks were exposed to multi-phase metamorphosis and tectonic deformation during the hercynic and alpine orogeny. Schistosity formed as a result of intensive shearing strain in the granite body. The posterior cooling of the rock was associated with formation of younger fracture systems.

Detailed structural analysis of collected surface and subsurface data identified more than ten individual discontinuity systems (KEUSEN et al. 1989) which can be classified into the following groups:

- Schistosity S: principal planes of weakness in the granite massif
- Fractures K
- Lamprophyre contacts L
- Alpine tension joints ZK

The spatial relation of the various systems is shown schematically in a block diagram in Fig. 1.

Several of the systems identified cannot, however, be distinguished properly in the field since they show a great variability in their orientation (i.e. in azimuth and dip) and overlap each other (example: principal schistosity S2 and shear planes S1).

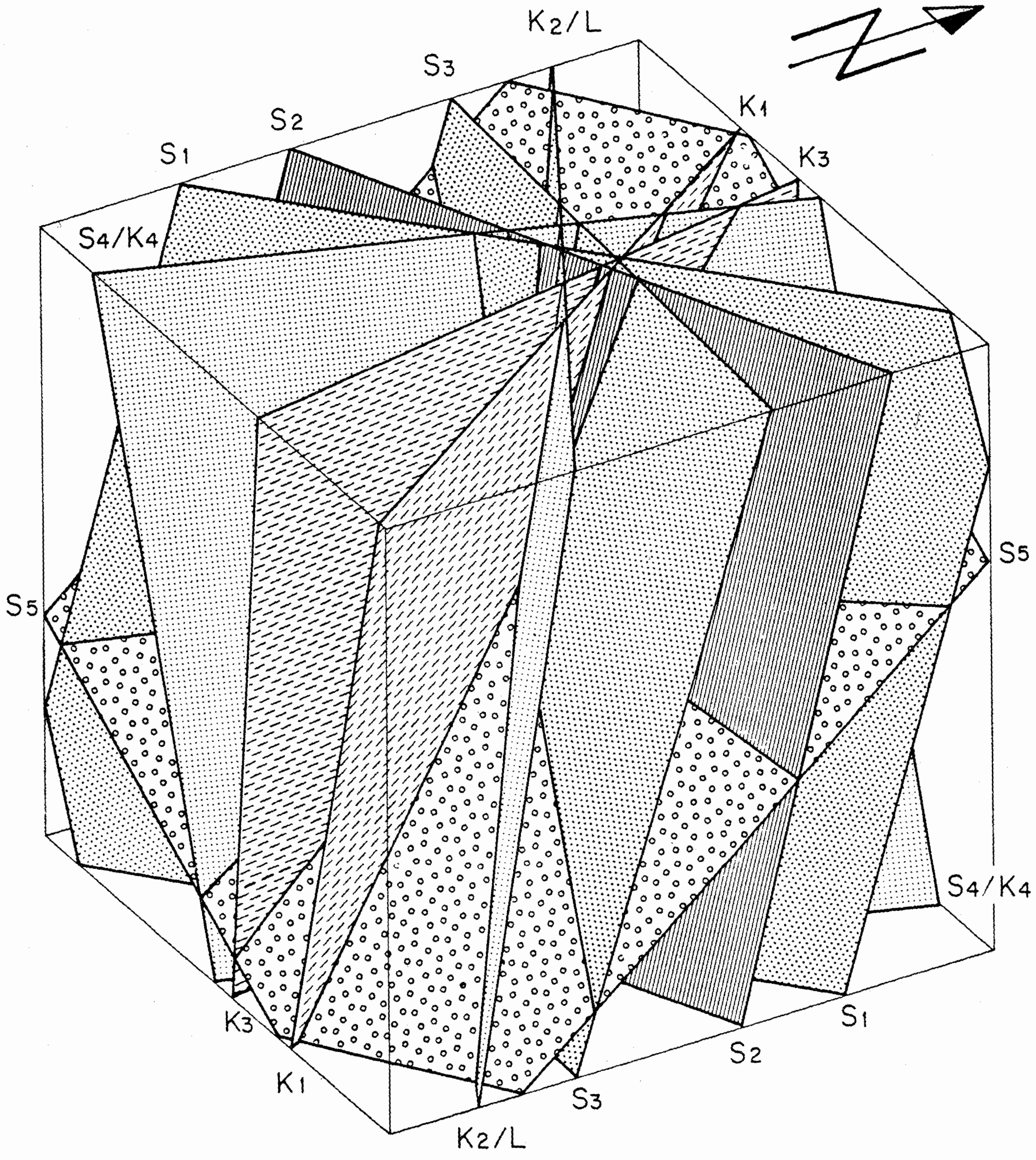


Fig. 1: Block diagramm of the dominant structures in GTS area (KEUSEN et al. 1989, Fig. 33)
S: schistosity-related systems
K: joint systems
L: lamprophyre

The dominating systems observed in GTS tunnels and oriented cores from GTS boreholes are by far the shear planes S1 + S2, followed by the K2 + L family, shear planes S3 and fractures systems K1 and K3. A different picture is obtained at the ground surface when considering the large-scale structural pattern. The region of the Juchlistock proves to be dominated by two systems only which have a distinct impact on the morphology of the rock surface (KEUSEN et al. 1989, Fig. 39). The mountain slopes are dissected by a rhomboidal pattern of two discontinuity sets. The dominant one corresponds to the shear planes S1 & S2, whereas the second set can be attributed to the fracture system K2. The morphologically conspicuous features correspond to prominent shear zones of a few meters' width. A major fault zone with a thickness of approximately 130 m was observed in the access tunnel beneath the Bächlisbach, approximately 250 m south from Gerstenegg portal (see Fig. 6).

2.2 Hydrogeology

In low-permeable fractured granite the movement of groundwater is virtually limited to individual more or less planar discontinuities. This can be clearly observed in the machine-excavated laboratory tunnel. Based on long-term observations of the tunnel walls and on results of packer tests performed in the GTS boreholes, the water circulation can be assigned to only a few planar systems.

The prominent water-bearing structures are the lamprophyre contacts L (related to system K2), shear zones of system S1+S2 and shear planes S3. The short horizontal tension joints were also found to be water bearing. This is explained by their genetic association with lamprophyre contact zones, the open tensile cracks being a result of differential deformation behaviour of ductile lamprophyre and brittle host rock respectively. The tension joints are thus considered as a secondary flow path. All water-bearing systems are characterized by their steeply dipping fracture sets. This pattern results in a pronounced subvertical hydraulic anisotropy of the granitic massif.

3 MODELING APPROACH

3.1 The Model Hierarchy

The applied concept consists of a hierarchic sequence of finite element models of decreasing size and thus increasing resolution.

On the first level a "regional model", which follows natural boundaries and extends over an area of 30 square kilometres, describes the groundwater flow in the alpine massifs surrounding the test site. The boundaries were chosen sufficiently remote in order to include natural boundaries and to reduce their influence on the head distribution in the near field of the GTS. Although many fracture systems were recognized in this area (Fig. 1), only the hydraulically significant ones (according to 2.2) were considered in the model and summarized into main fracture systems. In the regional model two main fracture systems (S, K) were distinguished.

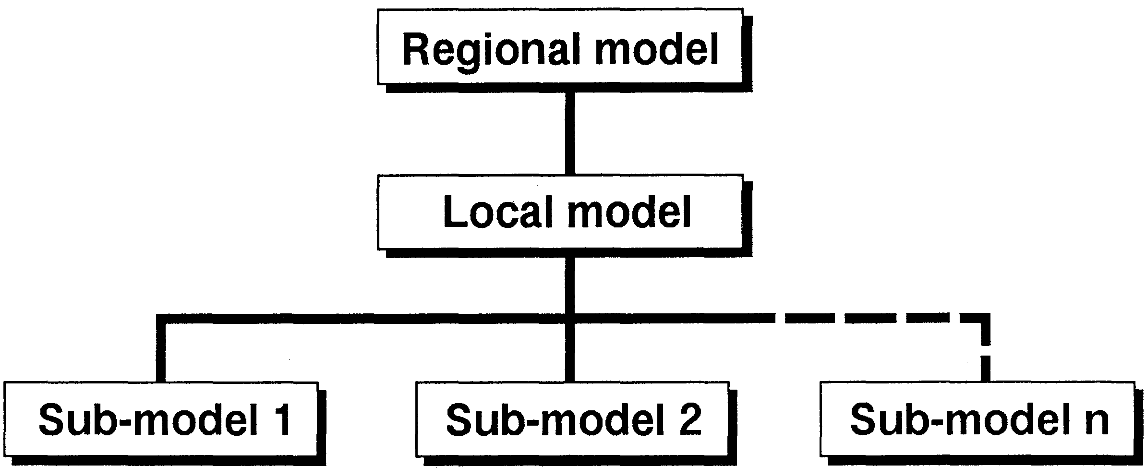


Fig. 2: The model hierarchy of project MOD

Since these features are all tilted, a special mesh generation procedure had to be applied. Two horizontal meshes, topologically identical but with a relative displacement reflecting the inclination of the two main fracture systems, were created. For an accurate reproduction of the layout at the GTS level, a third 2-D mesh was generated at this elevation to define the location and direction of the geological structures (Fig. 3).

On the second level the "local model" includes in detail the underground structures of the facility as well as fractures and shear zones out to a suitable distance where boundary conditions are supplied by the regional model (Fig. 4).

Due to the finer discretization of the mesh required for better resolution close to the GTS, a large number of finite elements were generated. In order to economise computer time during calculation a substantial number of the peripheral elements were "condensed". This procedure involved combining several small elements into one larger element with the same hydraulic properties as in the zones where no special resolution was required (see also Chapter 7.1).

The third and final level consists of very detailed "sub-models" which are tailored to the specific requirements of the individual experiments and take their boundary conditions from the local model. The development of these sub-models is not part of the Project MOD.

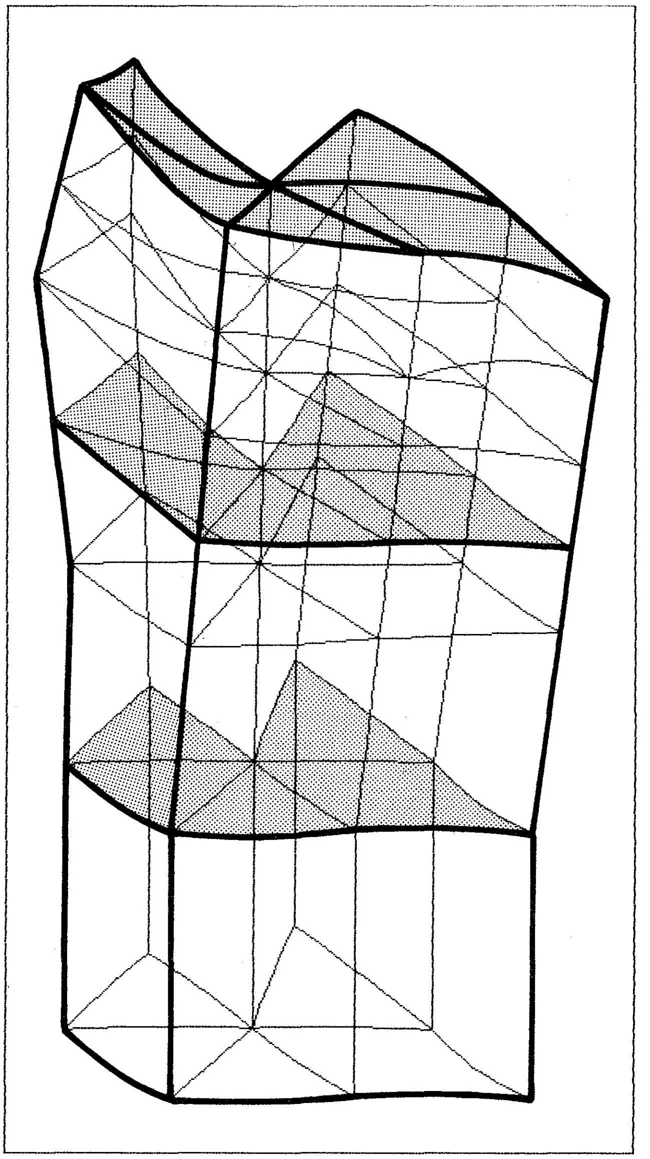


Fig. 3: Detail of the 3D-mesh with accentuated planes

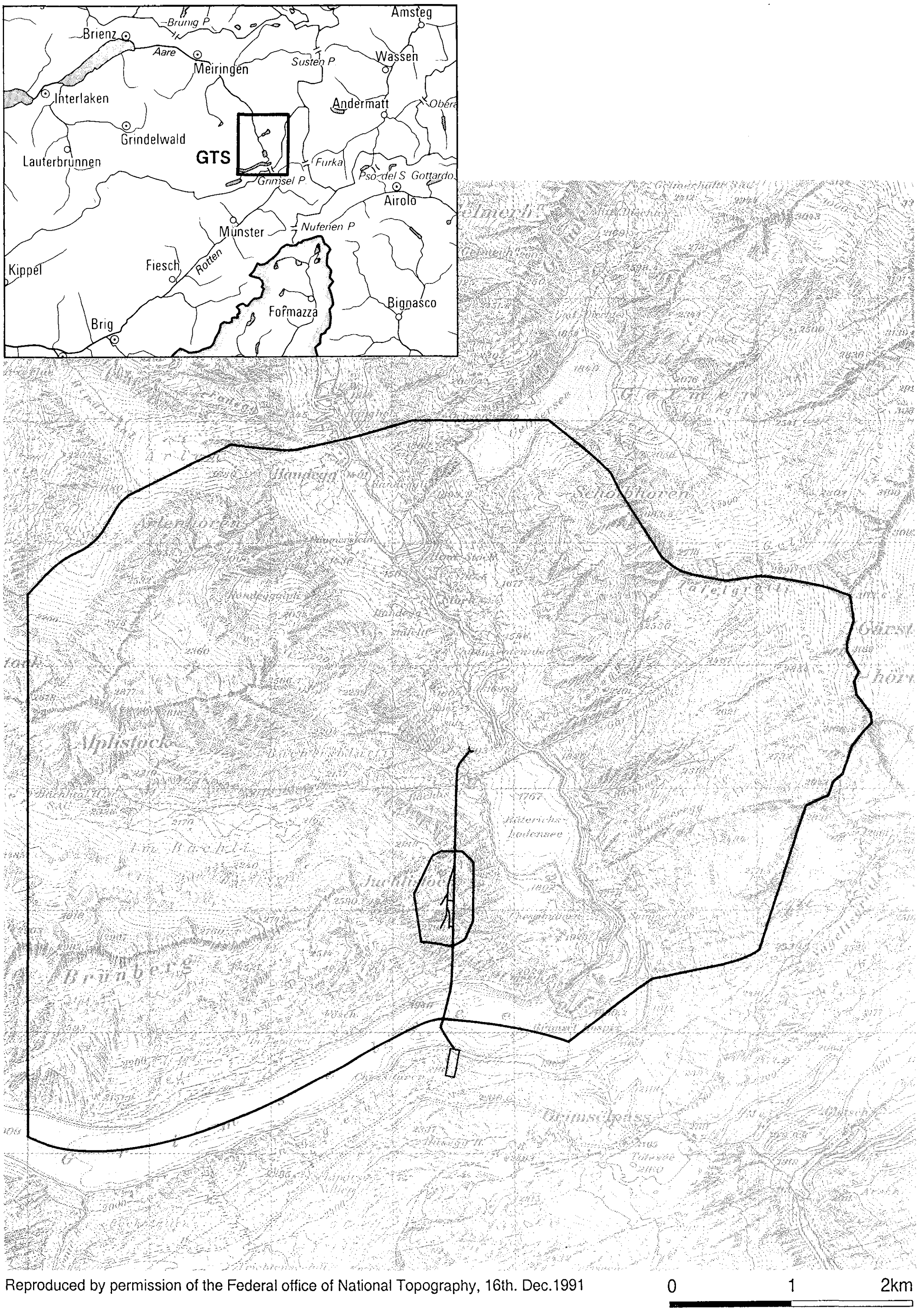


Fig. 4: Grimsel area with underground structures and countour lines of the regional and the local model, Scale 1:50'000

3.2 Concept of the FE Modeling

The principal procedure of the groundwater modeling is shown as a flow chart in figure 5. The sequence can be considered in three main parts. Firstly the preprocessing phase involves all relevant information to satisfy the criteria of the conceptual model, i.e. knowledge of the geologic and hydrogeologic situation, information on the topography and the groundwater table as well as on boreholes and structures. This part is characterized by the transformation of this knowledge into a model-conforming state.

The second part involves the implementation of the numeric model. In Project MOD, the finite element code FEM301 (KIRALY 1985) is used to compute the steady state saturated water flow in an equivalent porous medium, under the assumption of a constant specific weight of the flow phase (fresh water). For defining the 3-D mesh, the code uses an element and a coordinate file. The hydraulic properties (hydraulic permeability, porosity) of the hydrogeologic formations as well as the required boundary conditions are prescribed by a parameter file. The output is a result file which assigns a hydraulic head value to every nodal point of the mesh. For all nodal points with prescribed head (hydraulic potential) the code calculates an inflow and an outflow respectively, which is representative for the vicinity of the nodal point concerned.

In the third part (post-processing phase) the results are visualized by a finite element display code (FED) or analysed with additional codes for the determination of water flow and flow path respectively (TRACK).

3.3 Methodology of Calibration

3.3.1 General Approach

Starting from the observation of a natural phenomenon, an adequate conceptual model of the physical behaviour of this phenomenon is able to fit this observation. If the divergence between observation and calculations is negligibly small, the assumptions made in the conceptual model may be confirmed and predictions for these types of observations are possible.

The aim of calibration is to find a set of parameter values which yields the best simulation results. Usually the best simulation is defined as the one that yields the minimum sum of the squared differences between measured and calculated values. Since the observations are generally of variable accuracy due to instrumentation set up or the number of repetitions of the measurements, they have to be characterized by a weight. This weight is often defined as being proportional to the reciprocal value of the standard deviation of the measurements.

The core of the methodology for calibration is the definition of an objective function (CARRERA & NEUMANN 1986) which contains the most relevant hydrogeological quantities. For hydrogeological models extending over several hundred metres, these can usually be expected to comprise

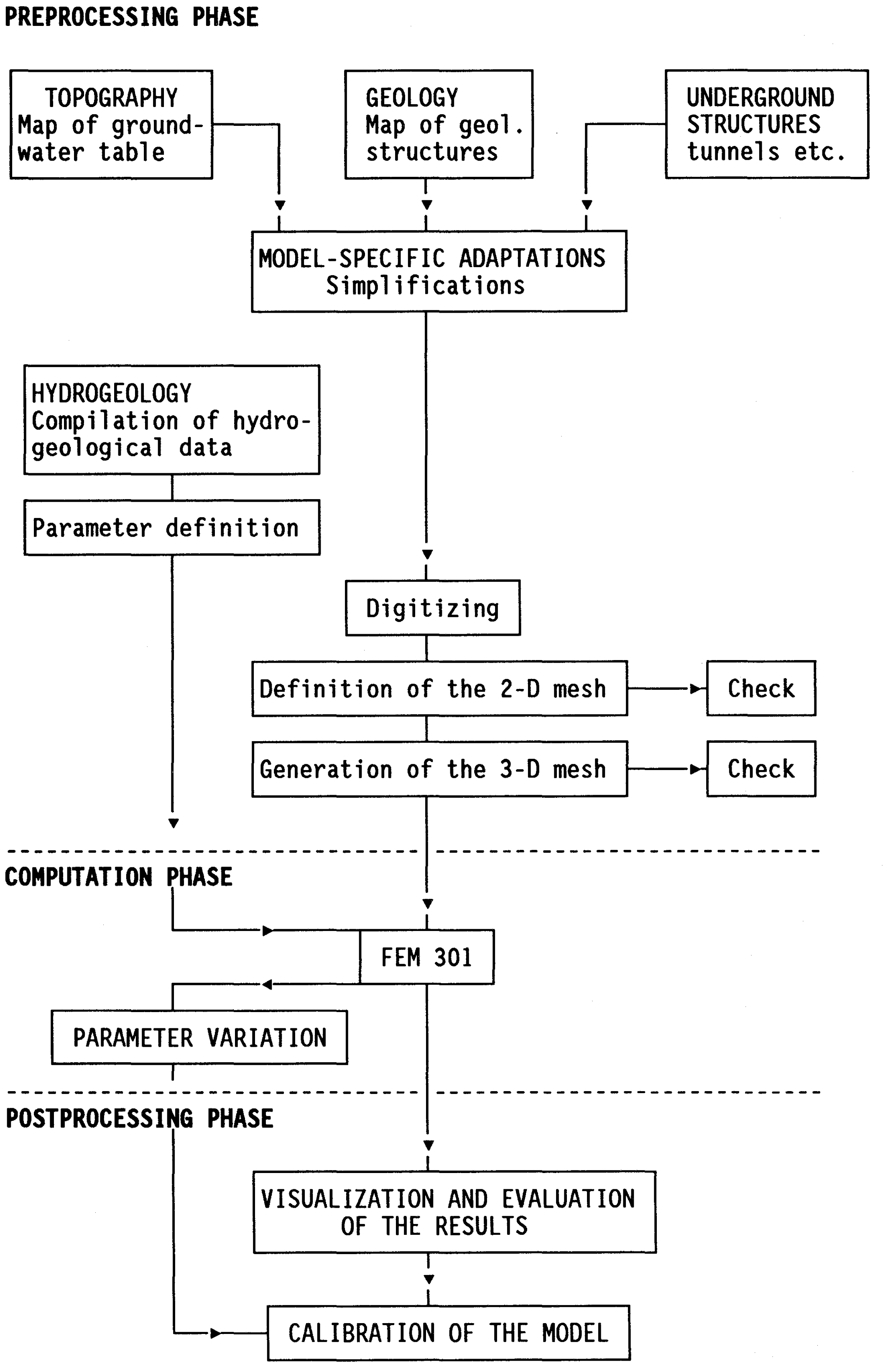


Fig. 5: Flow chart of the numerical groundwater modeling

head and flux measurements as well as hydraulic conductivities and transmissivities of the most relevant hydrogeological features.

It has to be emphasized that only head and flux can be measured directly by instrumentation. Hydraulic conductivity or transmissivity can only be determined by indirect measurement procedures (e.g. fluid logging). For this reason the head and flux measurements are of first interest for calibration procedure.

Some general remarks about head and flux measurements in this context should be mentioned:

a) Head Measurements

The simulation of the head field by a steady state model requires that the data also represents steady state conditions. Therefore, only head measurements with well documented values, preferably with an indication of the error standard deviation and of the observed pressure recovery (complete or not), should be used for calibration. The assignment of the measured heads to the corresponding nodal points of the model FE is usually possible only with uncertainties. In the vicinity of underground structures the hydraulic gradients are large and long test intervals prove to be unsuitable for calibration.

In a fissured host rock the head in a measurement section is strongly influenced by the discrete water inflow. If the location of the inflow point can not be determined or if the packed-off section shows several water-conducting features the unequivocal assignment of the measured head is not possible.

b) Water Flow into the Tunnel

The general judgement of the flow field is based on the fact that at each nodal point of a numerical model with prescribed head the water flow is calculated. The integration of underground structures into a model requires boundary conditions along these structures. Assuming that these inner boundary conditions are given by fixed heads, fluxes at each nodal point will be calculated and the summation of all these fluxes should be compared with the observed total inflow into the underground structures.

Therefore the calibration of the water flow is easier to achieve if the observed water flow is assigned to a region of the model which contains a representative range of the host rock (referring to the representative-elementary-volume-concept, see e.g. BEAR 1979). Due to the linear relationship between fluxes and permeabilities, the hydraulic permeabilities or transmissivities can be estimated easily. Fluxes along boreholes or within packer test sections can only be simulated if enough nodes were provided and fixed heads were defined.

If the outside boundary of the hydrogeological model reaches the surface, the calculated or prescribed flow rate may be compared with the anticipated infiltration rate due to the precipitation and snow melt, reduced by the evaporation and the surface run-off. The infiltration rate is not a measured quantity and this comparison gives only a very rough criterion, but it can be used as a plausibility check to eliminate assumed permeabilities which require infiltration rates greater than the precipitation. Because of the fixed heads at the boundaries the overall transmissivities can not be set arbitrarily to reproduce the measured fluxes.

3.3.2 Objective Function

The most relevant hydraulic quantities for simulation of a steady state and saturated flow regime are the hydraulic heads and fluxes. Therefore the defined objective function (J) contains two terms which take account of the residuals of heads (h) and fluxes (Q). The residuals are defined as differences between calculated and measured values.

To consider the different weights of measured values, the residuals are divided by an estimated error value and to prevent negative and positive residuals cancelling each other, the weighted residuals are squared (CARRERA & NEUMANN 1986).

$$J = \sum \frac{(h^{o} - h^{*})^{2}}{(2\sigma_{h})^{2}} + \sum \frac{(Q^{o} - Q^{*})^{2}}{(2\sigma_{Q})^{2}} = J_{h} + J_{Q} \qquad (1)$$

where:

- h^{o}, h^{*} mean calculated and measured head [m])
- Q^{o}, Q^{*} mean calculated and measured flux [$m^{3} \cdot /s^{-1}$]
- σ_{h}, σ_{Q} mean estimated prior standard deviation of head and flux respectively

The main aim of calibration comprises finding a model parameter set which gives the smallest sum of weighted residuals, in other words, minimizing the objective function (J) for the selected conceptual model. In order to keep the number of necessary runs small the relevant parameters have first to be defined. As described above, the transmissivities of the fracture systems have a dominant influence on the flow field while the hydraulic conductivities of the lamprophyres and the granite are less significant. In Section 6.3, an application of this proposed calibration method will be demonstrated and discussed.

Adopting the maximum likelihood approach (by minimizing J) we make the implicite assumption that the conductivity (or transmissivity) values of the various "features" (i.e. matrix at various levels, the various fracture systems etc.) have unknown but constant values. If within a block or zone there exists a heterogeneous pattern, this will affect the standard deviation of the measured head, flux, or initial estimates of K and T. The value that we will estimate from the data set should then be considered as the effective (or mean) value of K or T for that block or zone respectively. Recognizing the above factors also leads to the conclusion that we should not expect to achieve complete match among the measured and calculated head values - except due to coincidence. In other words, the value of J will practically never become zero.

3.3.3 Optimization Techniques

Two general approaches can be outlined for obtaining the most optimal model parameter set by minimizing the objective function J, as defined in Eq. (1). The first is a heuristic trial-and-error approach, involving a search in the parameter space. The second is a nonlinear regression approach which utilizes information about the sensitivity of the objective function to the unknown parameters. Details of these two approaches are briefly presented below.

In the trial-and-error approach, the first step is to define the feasible range (i.e., minimum and maximum values) for the unknown parameters. This range is then discretized into a search grid in some empirical fashion. For example, a search step for transmissivity could be one or half an order of magnitude. Subsequently the objective function is evaluated for each point in the parameter space using a systematic or a random procedure. The point corresponding to the minimum value of J is taken to be the set of optimal parameters. Such a trial-and-error approach is easy to implement, and may be the only practical alternative for large-scale models due to computational limitations. However, unless the parameter space is properly defined and discretized, the optimal parameter set may not be found.

The nonlinear regression approach, although computation intensive, seeks to minimize the objective function by progressively and iteratively refining the parameter set. At each iteration, the parameters are updated in the direction along which J is reduced. This requires information regarding parameter sensitivities, which adds to the computational burden. However, the advantages of such an approach are:

(i) at least a local minimum for J can be found, and

(ii) parameter uncertainties can be quantified, at least in an approximate manner.

In the calibration of the local model GTS, described in Section 6.3, the trial-and-error approach was utilized for computational convenience.

4 DATA BASE

4.1 Model Geometry

The basis for the geometric layout of the model grids (regional and local model) comprises two maps of geologic structures with the scale of 1:10'000 for the regional model and of 1:2'500 for the local model respectively. These maps were based primarily on the interpretation of aerial photographs. In addition, a horizontal section at the level of 1730 m a.s.l., which takes into account the geological structures in the area of the main access tunnel (KWO-Tunnel) was generated. All maps were prepared by GEOTEST Ltd., Zollikofen, Nagra's geological consultant for the GTS Project. A vertical profile (Fig. 6) along this tunnel also shows the possible correlation of surficial geological structures with the corresponding features at the level of the main access tunnel. In this context, a fundamental problem arose when the knowledge of a relatively small area was to be extrapolated to a wide area of more than 30 square kilometres. This problem generally arises when two observation domains with different scales are considered. The correlation between the observed geological features within the tunnel and at the surface shows that only the most important shear zones in the access tunnel can be assigned to pronounced morphologic features at the surface.

The large-scale layout of the surficial geological features in the Juchlistock area has a much simpler pattern compared with the complex geometry observed in the underground structures and associated drillholes. At the surface, 2 to 3 main shear zone systems were recognized. Because of this fact, the geologic features at the level of the tunnel had to be summarized into the same number of shear zones to enable a consistent assignment within the geologic system.

4.2 Hydraulic Conductivities / Transmissivities

The assignment of the hydraulic properties to the hydrogeological units is based on review of the available data base. Measurements of hydraulic conductivities were taken from packer tests in the first exploration boreholes performed from the main access tunnel (NAGRA 1985, Tab. 9) and from in-situ experiments (migration experiment, ventilation test, fracture system flow test). The interpretation of these experiments shows that the water flow is concentrated in discrete fractures. The corresponding measured transmissivities manifested a range of 10^{-9} m^2/s to 10^{-6} m^2/s. The undisturbed rock matrix is characterized by low permeabilities: based on laboratory experiments the hydraulic conductivities are assumed to be in the range of 10^{-10} to 10^{-12} m/s. Zones in the crystalline matrix with locally higher permeabilities are confined to hydrothermally leached inclusions.

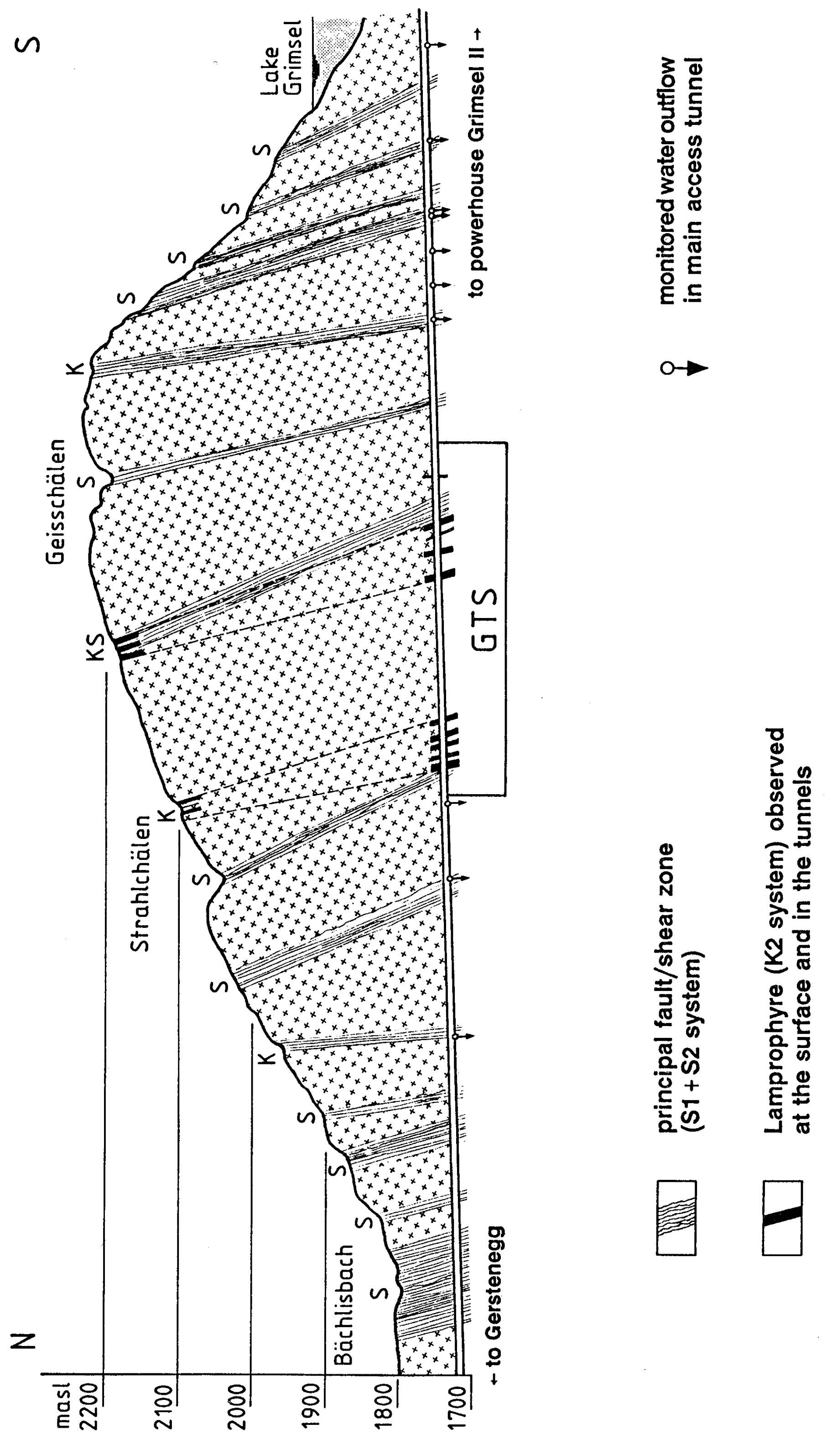


Fig. 6: Vertical geological section along the main access tunnel showing principal tectonic structures basically considered in regional model (after KEUSEN et al. 1989)

4.3 Fluxes

Due to the different scale of each model (i.e. regional and local), different flow data sets are used for model calibration. Flow measurements taken along the main access tunnel (see KEUSEN et al. 1989, attach. A7) are used for the regional model where internal boundary conditions were imposed, while flow data coming from various discrete locations in the GTS tunnel are used for the local model.

Because of the larger number of observed seepage locations compared with the limited number of discrete potential outflow points in the models, the simulated fluxes into the underground structures are integrated over a defined tunnel section and compared with the corresponding measured fluxes . For calibration of the regional model using flow data, the main access tunnel was divided into three water-bearing sections of several 100 m length each (see Section 5.4, Table 6), while in the local model the GTS tunnel was divided into five zones (Fig. 7), in each of which the calculated and measured flows were compared. An expected error magnitude was assigned to each flow measurement. For lower flow measurements, the relative effect of evaporation will be greater. Therefore, these measurements are considered to be generally less accurate.

Figure 7 shows the five zones within the GTS tunnel system as defined on the basis of available flow measurements. In each zone, at least one reliable flow measurement is available. Four significant measurements are available at the experimental test sites BK, VE, WT and MI, and, since the total outflow from the entire GTS tunnel system (Q_{total} in Fig.7) is known, a fifth residual zone (RES1+2) can be defined which represents the remaining part of the GTS tunnel system. The difference between the total measured outflow (Q_{total}) and the sum of the four individual fluxes ($Q_{BK} + Q_{VE} + Q_{WT} + Q_{MI}$) is assigned to this residual section. In this manner, the resulting total outflow is indirectly treated as a flow measurement at a specific location.

4.4 Hydraulic Heads

Since 1980, hydrostatic pressure has been monitored systematically with six exploration boreholes, drilled subhorizontally from the main access tunnel prior to the excavation of the GTS (boreholes SB 80.001-80.006, see layout map at the beginning of this report). Considerable differences in pressure have been observed in parallel boreholes at a distance of only 80 to 100 m from each other (NAGRA 1985, Fig. 35). These observations give no indications about either the transient state of the pressures or the relationship to the levels of the Lake Grimsel and Lake Räterichsboden respectively. Therefore, no hydraulic heads were considered for calibration of the regional model. On the other hand, for the calibration of the local model, hydraulic heads are available for the following three investigation sites: Ventilation test (VE), rock stress measurements (GS), and fracture-zone investigation (BK). Pressure build-up data from the VE site are considered to represent the most accurate source of this data set.

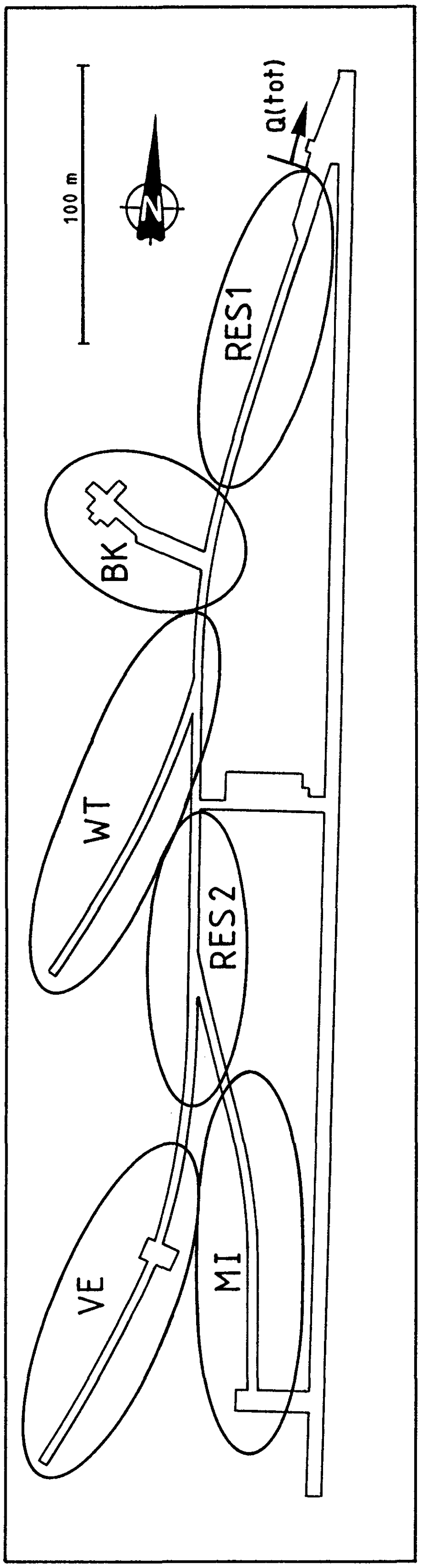


Fig. 7: Division of the GTS tunnels into five zones for comparison of measured and calculated fluxes (RES1+2 = residual section)

5 REGIONAL MODEL

5.1 Conceptual Model

5.1.1 Model Grid

The regional model covers an area of approximately 30 km^2 (Fig. 4). The considered region is characterized by a strong relief with the surface elevation showing a range between 1'400 and 2'900 m a.s.l. Vertically, the model extends from the surface down to an elevation of 500 m a.s.l. The layout of the horizontal mesh is presented in Fig. 8. It considers the main topographic features, such as valleys, ridges and lakes. Its geometry, however, is clearly dominated by the rhombohedral pattern of the two prominent discontinuity systems in this region. Both directions represent a large-scale anisotropy in the granitic massif of Juchlistock and adjacent areas and are referred to as the dominating system S (main schistosity S1 + S2) and the system K (associated discontinuities K2 + 1) respectively. These planar features are reproduced in the grid by 2-D elements, their thickness being assumed as negligible with respect to their spatial extent. As an exception, the Bächlisbach fault, a major feature with significant thickness was represented by 3-D elements. Additionally, subvertical 1-D elements were included in the grid at some prominent intersections of systems K and S in order to reproduce the local increase of permeability. Also considered in the horizontal grid layout is the alignment of the main access tunnel to the power station Grimsel II (and to the GTS). Other tunnels of the hydropower plant which may affect hydraulic conditions of surrounding rock are not modeled explicitly but represented by fixed potential values at corresponding nodes in the grid.

The vertical structure of the grid is shown in Fig. 9. The model is divided into six layers, two above the level of GTS and four below. Each layer can be assigned an individual material property to simulate depth-related decrease of hydraulic conductivity or transmissivity respectively. Since all considered planar dicontinuities are inclined, the 3-D grid had to be generated by means of tilted columns. This procedure requires first the construction of two horizontal grids with identical topology at the bottom and the top of the model. Identical topology means that each bottom mesh element is represented in the surface mesh with the same geometry in order to ascertain the continuity of the 3-D oblique columns. This implies that the tectonic features defined at the topography surface cannot pinch out or branch into minor structures in the interior of the model grid. Further, all fractures belonging to the same system are assumed to be more or less parallel to avoid their intersection at deeper levels of the model.

The task of reproducing a correct geometry of the principal features in the horizontal plane of the GTS required the definition of an additional horizontal 2-D mesh at this level. Since the geometric pattern of the shear zones in the GTS observation area cannot be easily correlated to the surface, significant simplifications of the geometry were required for the sake of identical mesh topology at both the GTS level and the model surface.

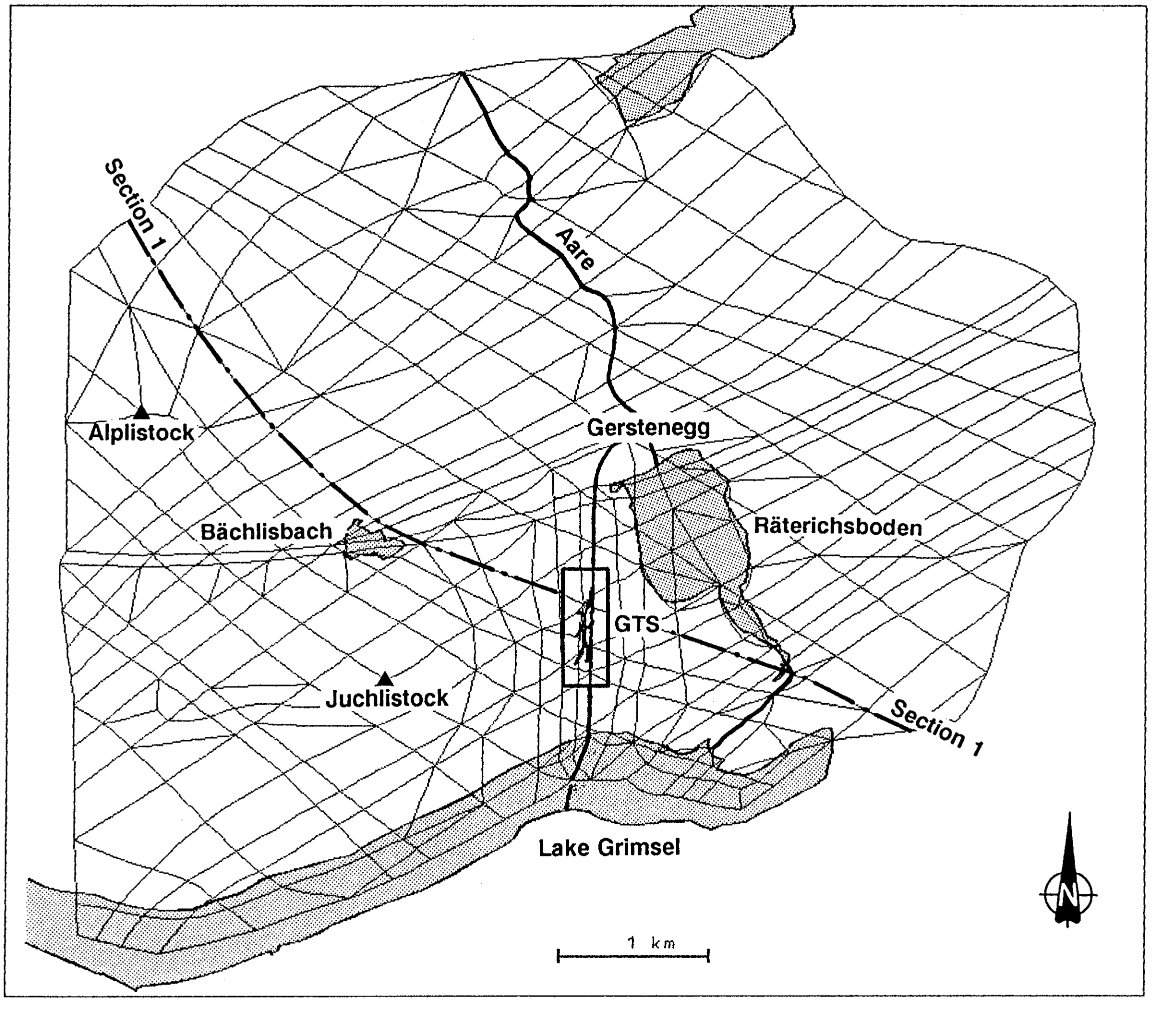


Fig. 8: Regional model GTS: horizontal discretization of the grid

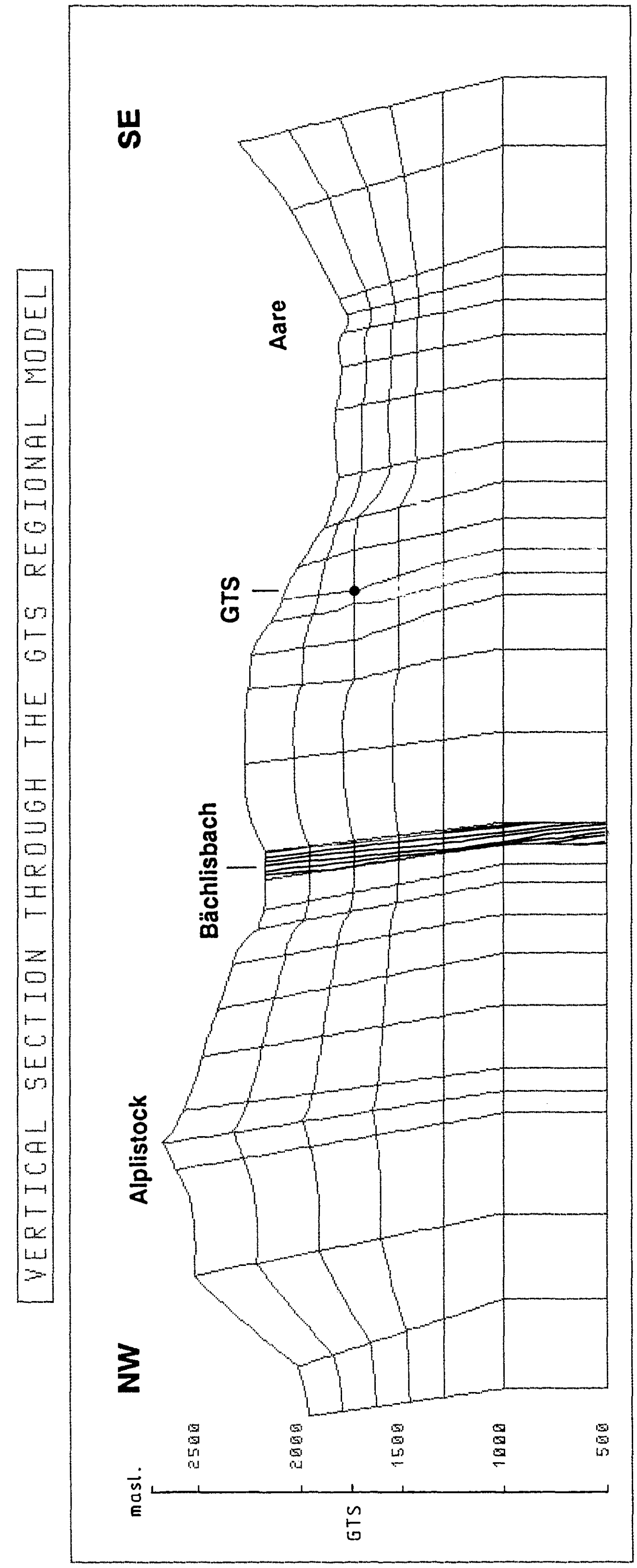


Fig. 9: Regional model GTS: Vertical grid along section 1

5.1.2 Boundary Conditions

The conceptual model assumes impermeable boundaries for the bottom and the lateral model walls (no fluxes across the boundaries). For this purpose, the lateral limits of the model were established along such areas where prevailing vertical groundwater flow or flow direction parallel to the boundary respectively can be expected (e.g. beneath the lakes, valley bottoms and mountain ridges). The top surface of the model is defined by the groundwater table according to the adopted concept of saturated equivalent porous media (Dirichlet condition). For the purpose of modeling, the groundwater table is assumed to coincide with the topography surface, i.e. each nodal point is assigned a head corresponding to the ground elevation. This approximation is justified for the generally low-permeable granitic rock but it is less realistic for the more permeable discrete features, such as shear zones and faults, where it produces higher fluxes within these structures and enhances the effects of surface topography on the potential distribution. However, both these effects are of no great significance at the depth of the GTS, 450 m below the surface, as can be verified by comparing the simulated and observed inflow rates into the tunnel and hydraulic gradients respectively. On the other hand, it should be emphasized here that under different site-specific conditions (e.g. higher permeable materials), such a simple approximation would no longer be admissible and would need to be replaced by an estimated effective groundwater level as the top surface boundary of the model.

5.1.3 Hydrogeologic Units

Besides the low-permeable granitic matrix, the regional model includes the two main fracture systems K and S. These principal fracture systems, together with the Bächlisbach fault zone, are considered to govern the large-scale hydraulic anisotropy of the massif. Both considered systems K + S are characterized by their water-bearing appearance in the tunnels and boreholes and by large lateral extent at the surface respectively. System K incorporates also the lamprophyre contacts L and is, therefore, considered to be more permeable than system S. For the purpose of simulating the effect of intermittent fractures (i.e of laterally limited extent), most planar features were divided into two hydraulic segments. By reducing the transmissivity of one given section, parts of the fractures can be hydraulically deactivated. As mentioned above, some prominent steep intersections of planar shear zones were reproduced as an individual hydrogeologic unit (1-D elements). To summarize, the model is composed of the following hydrogeologic units: Block matrix (homogeneous-porous), Bächlisbach fault zone, planar fracture system S and K (each divided in two sections) and linear intersection of S and K.

Additionally, the layered structure of the model (Fig. 9) allows a vertical zoning of hydraulic properties for the mentioned units. Hence, the established 7 hydrogeologic units can be assigned totally 42 different permeability classes when considering all options.

An overview of the hydrogeologic units considered is given in Table 1:

K-class No.	Symbol	Unit	Dimension of FE
1 - 6	GR	granitic matrix	3-D
11 - 16	BS	Bächlisbach Fault	3-D
21 - 26	K	main system K2 & L	2-D
31 - 36	S	main system S1 & S2	2-D
41 - 46	K′	segment of K	2-D
51 - 56	S′	segment of S	2-D
61 - 66	KxS	intersection of K&S	1-D

Table 1: Hydrogeologic units of the regional model

5.2 Parameter variation

The sensitivity study performed with the regional model involved the variation of hydraulic properties of the considered tectonic structures and the simulation of steady-state groundwater conditions in the undisturbed massif. Within the scope of model calibration, several parameter variations were carried out on a small partial model extracted from the regional model in the water-bearing southern section of the main access tunnel. The resulting best parameter set was then included in the main model to represent the actual calibration case.

The summary of the model runs performed is presented below:

Run No.	Parameter Variation
R01	Base case (best-guess values)
R02	Undisturbed conditions, no tunnels
R03	K/S fractures high permeability
R04	K/S fractures low permeability
R05	K/S fractures not continuous
R06	Matrix only (isotropic)
R07	BS fault high permeability
R08	BS fault low permeability
R09	"Calibration" case

The **Base Case** (Tab. 2) was established as the most probable configuration of parameters. The assigned hydraulic properties are deemed to represent the "best-guess" data that could be estimated at the conceptual stage of the model. The assumed basic parameter set is presented in Table 2.

The second **Run R02** simulated undisturbed hydraulic conditions within the Juchlistock massif by "switching-off" the existing tunnels. The objective was to simulate the steady state groundwater flow regime existing prior to the construction of underground structures and to determine the extent of influence of the modeled tunnels on the potential distribution.

The next four model runs were dedicated to the estimation of the hydraulic significance of the discrete fracture systems K and S:

Run R03 ("K+S high", Table 3) considers high permeability of the tectonic features. The transmissivities of both principal systems K and S were increased by a factor of 10 with respect to the basic values.

Run R04 ("K+S low" Table 4) simulates an analogous reduction of transmissivities relative to the base case.

Run R05 investigates the impact of limited lateral extent of the fractures on the groundwater flow in the GTS area. Both fracture systems are disconnected hydraulically in the vicinity of the tunnel in order to suppress the effect of the large-scale anisotropy within the jointed granitic massif.

The extrem case of an isotropic rock matrix with no discontinuities at all is considered in **Run R06**.

A similar sensitivity analysis was performed on the observed fault zone of Bächlisbach (BS). Due to its large thickness and lateral extent, this feature represents a significant hydraulic inhomogeneity in the granitic massif. Since no field data are available for the estimation of its hydraulic properties, the parameter variations cover a wide range of uncertainty. **Run R07** ("BS high") simulates a drainage effect of the shear zone by increasing its hydraulic conductivity by factor of 100 with respect to basic assumptions. On the other hand, the **Run R08** ("BS low") considers its effect as a hydraulic barrier by reducing the permeability by two orders of magnitude with respect to the base case.

The final **Run R09** (Tab. 5) performed with the regional model represents virtually the calibration case. The parameter set adopted resulted from several calibration efforts which were undertaken with a small (and more flexible) partial "model box" in the southern part of the main model. In contrast to the "global" increase of transmissivities in run R03, this variation considers a selective and locally limited increase of T-values by differentiating individual segments of fractures.

LAYER No.	MATRIX K(m/s)	FAULT K(m/s)	2-D FRACTURE SYSTEMS T (m^2/s)				INTERS. (m^3/s)
	GR	BS	K	S	K'	S'	K x S
1	E-10	E-08	E-07	E-08	same	same	E-06
2	5E-11	E-09	E-07	E-08	as K	as S	E-06
3	E-11	E-09	5E-08	5E-09			5E-07
4	5E-12	E-09	E-08	E-09			E-07
5	E-12	E-09	E-08	E-09			E-07
6	E-12	E-09	E-08	E-09			E-07

Table 2: Hydraulic properties assigned to the base case R01

LAYER No.	MATRIX K(m/s)	FAULT K(m/s)	2-D FRACTURE SYSTEMS T (m^2/s)				INTERS. (m^3/s)
	GR	BS	K	S	K'	S'	K x S
1			E-06	E-07	same	same	5E-06
2			E-06	E-07	as K	as S	5E-06
3			5E-07	5E-08			E-06
4			E-07	E-08			5E-07
5			E-07	E-08			5E-07
6			E-07	E-08			5E-07

Table 3: Paramater variations in run R03 ("K & S high")

LAYER No.	MATRIX K(m/s)	FAULT K(m/s)	2-D FRACTURE SYSTEMS T (m^2/s)				INTERS. (m^3/s)
	GR	BS	K	S	K'	S'	K x S
1			E-08	E-09	same	same	E-07
2			E-08	E-09	as K	as S	E-07
3			5E-09	5E-10			5E-08
4			E-09	E-10			E-08
5			E-09	E-10			E-08
6			E-09	E-10			E-08

Table 4: Paramater variations in run R04 ("K & S low")

LAYER No.	MATRIX K(m/s)	FAULT K(m/s)	2-D FRACTURE SYSTEMS T (m^2/s)				INTERS. (m^3/s)
	GR	BS	K	S	K'	S'	K x S
1					5E-07	5E-08	E-05
2					5E-07	5E-08	E-05
3					E-07	E-08	5E-06
4					5E-08	5E-09	E-06
5					5E-08	5E-09	E-06
6					5E-08	5E-09	E-06

Table 5: Paramater variations in run R09 (local segments of K&S only)

5.3 Results

5.3.1 General

Graphic presentation of computed heads in the model is realized by the projection of equipotential lines onto selected vertical or horizontal sections through the model. To emphasize the effect of a considered parameter variation, head differences related to the base case can be plotted directly instead of equipotential lines.

The following description of the simulated groundwater flow regime in the model area is based on a horizontal section at the level of the GTS tunnels (elevation 1730 m a.s.l.) and on a vertical cross-section 1 running diagonally across the model from NW to SE (parallel to system K, see Fig. 8 and 9) respectively.

5.3.2 Base Case Conditions

The regional tendency of groundwater movement is depicted in the horizontal section in Fig. 10. The contours of the equipotential lines are conditioned by the surface relief. The massifs of Alplistock and Juchlistock in the western part and the Gärstenhörner in the eastern part can be distinguished clearly as the principal infiltration areas in the model. On the other hand, the Aar valley appears as the regional discharge zone, with the lowest discharge area within the model being located at Handegg at the elevation of 1'400 m a.s.l.

The alignment of the north-south oriented main access tunnel to the KWO power station Grimsel II is evident as a significant sink which generates steep hydraulic gradients in adjacent elements, particularly on the mountain side of the tunnel. The general groundwater flow in the model region is orientated towards the Aar valley, except for the southern slope of Juchlistock ridge which drains into the lake of Grimsel. Relatively low heads beneath the western part of the BS fault zone indicate a local drainage effect of this feature, which represents a direct hydraulic connection to the Aare.

The vertical head distribution and resulting flow directions are presented in Fig. 11. Vertical flow downwards can be observed beneath the identified infiltration areas, whereas the discharge area of the Aare valley is characterized by an upward flow. The intersected KWO access tunnels to Grimsel II (including GTS) and Grimsel I respectively are evidenced as distinct sinks. The highest hydraulic gradients towards the tunnel are formed in the principal direction of flow beneath the Juchlistock massif.

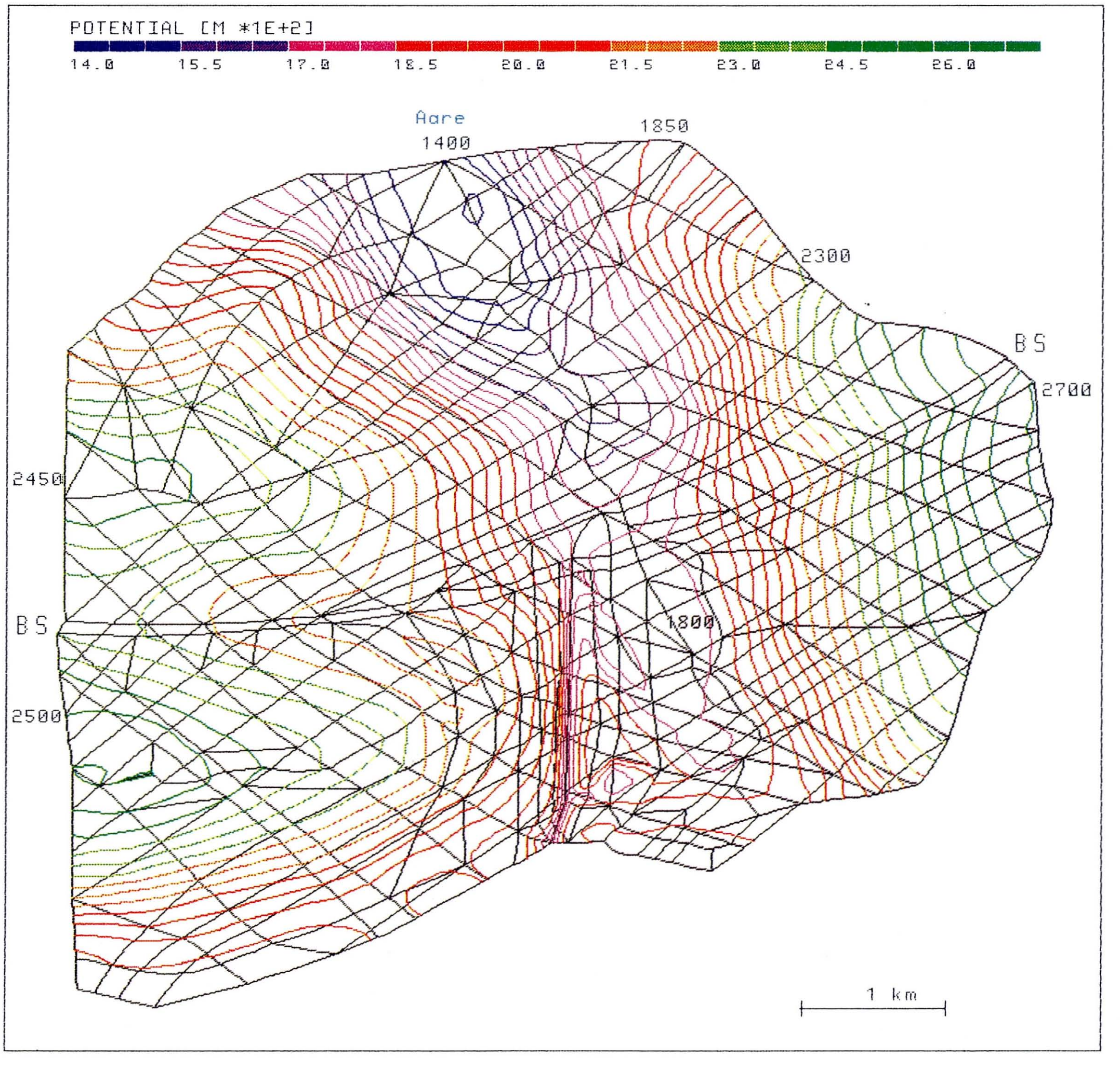


Fig. 10: Base case R01: calculated head distribution on a horizontal section at GTS level (elev. 1730 m a.s.l., top of layer 3)

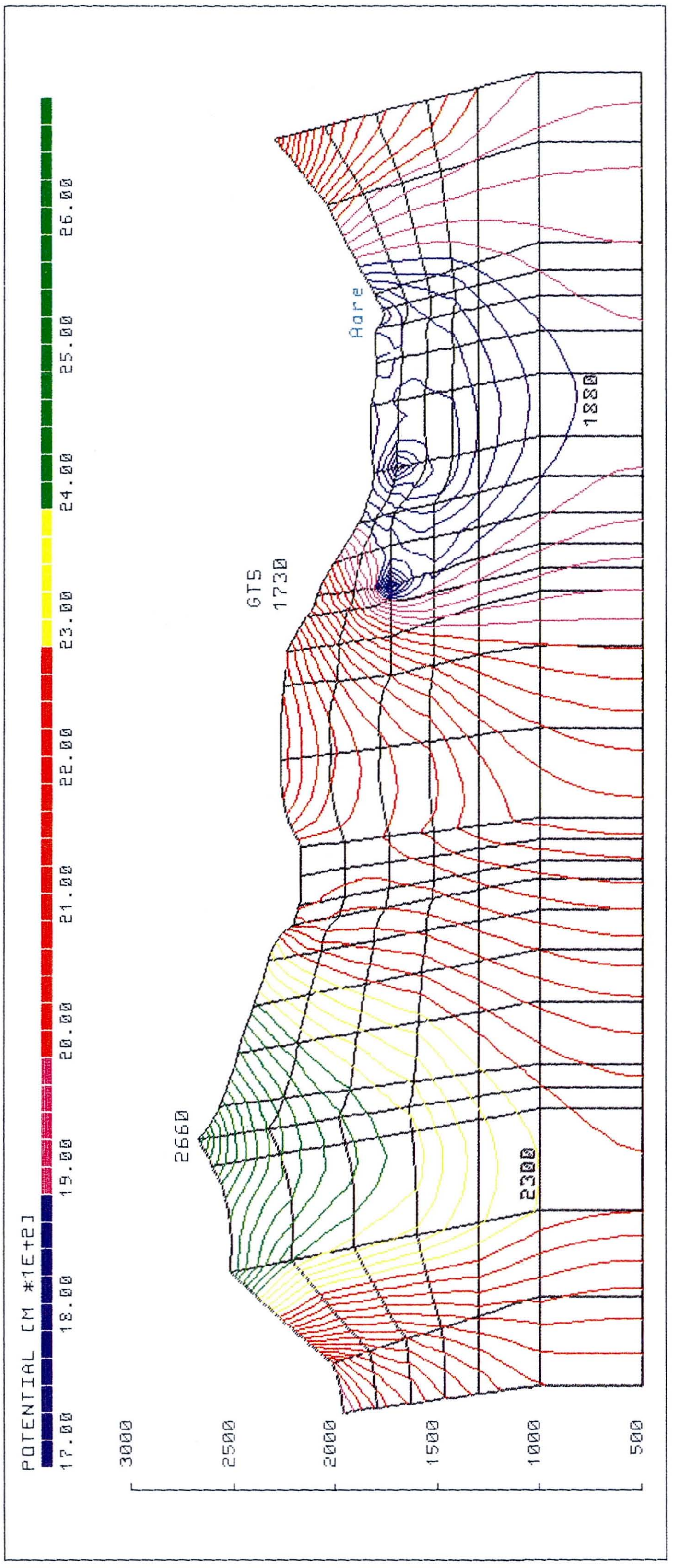


Fig. 11: Base case R01: Calculated hydraulic heads in section 1

5.3.3 Undisturbed Massif

The undisturbed groundwater regime (i.e. prior to the tunnel excavation) within the considered Juchlistock massif was simulated in run R02. Fig. 12 shows the vertical section with head distribution in the absence of tunnels. The direction of flow in the GTS zone is now governed by the infiltrations in the Juchlistock area and the drainage effect of the Aar valley. The simulated heads at the location of the GTS range between 2'030 m and 2'130 m a.s.l. These values correspond about to the highest hydrostatic pressure ever measured in the subhorizontal investigation boreholes drilled from the main access tunnel prior to the excavation of the GTS tunnel system (42 bar in SB 80.001 in 1981/82, see NAGRA 1985, Fig. 35).

To determine the impact of the tunnels on the simulated head distribution in the model, the resulting head differences between undisturbed condition (R02) and the base case (R01) are plotted in the horizontal section in Fig. 13. Besides the main access tunnel a lateral drift to the Aar valley, an old adit to Grimsel I, and a free-flow tunnel beneath the Juchlistock appear as "sinks" on the plot. The contours illustrate the lateral extent of tunnel effects on the potentials. Beneath the Juchlistock, a "sink" of 100 m difference can still be observed at 500 m distance from the main tunnel. Similar tendencies can be detected when comparing the vertical sections, where the heads are disturbed down to the bottom of the model beneath the main tunnel.

Thus the comparison of the base case conditions with the "no tunnels" szenario (representing for instance a backfilled and sealed repository) shows that - due to the rather coarse grid discretization of the regional model - the tunnels exert head disturbances within an unlikely large area of influence. This effects are of essential importance with regard to the boundary conditions to be provided for the local model. At the location of the envisaged boundary of the local model, the simulated head distribution in the base case still manifests a tunnel-induced disturbance of more than 100 m which is considered as being unlikely.

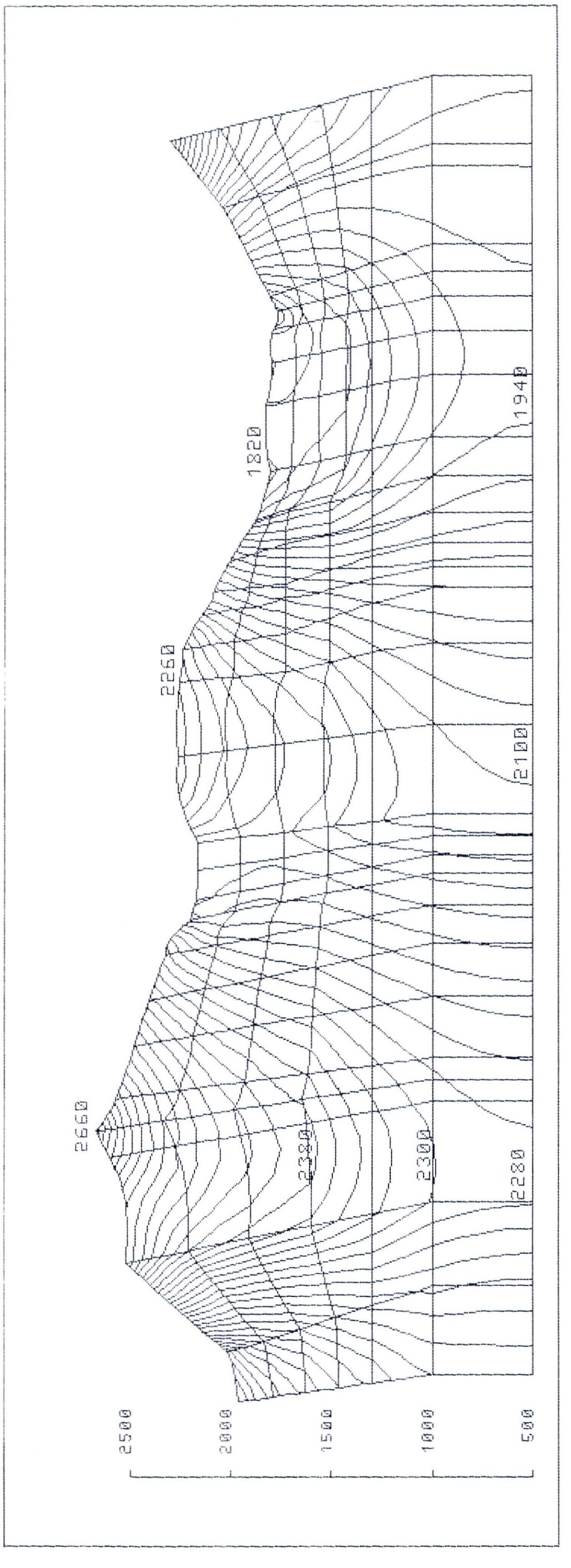


Fig. 12: Run R02: Calculated hydraulic heads in vertical section 1 ("no tunnels")

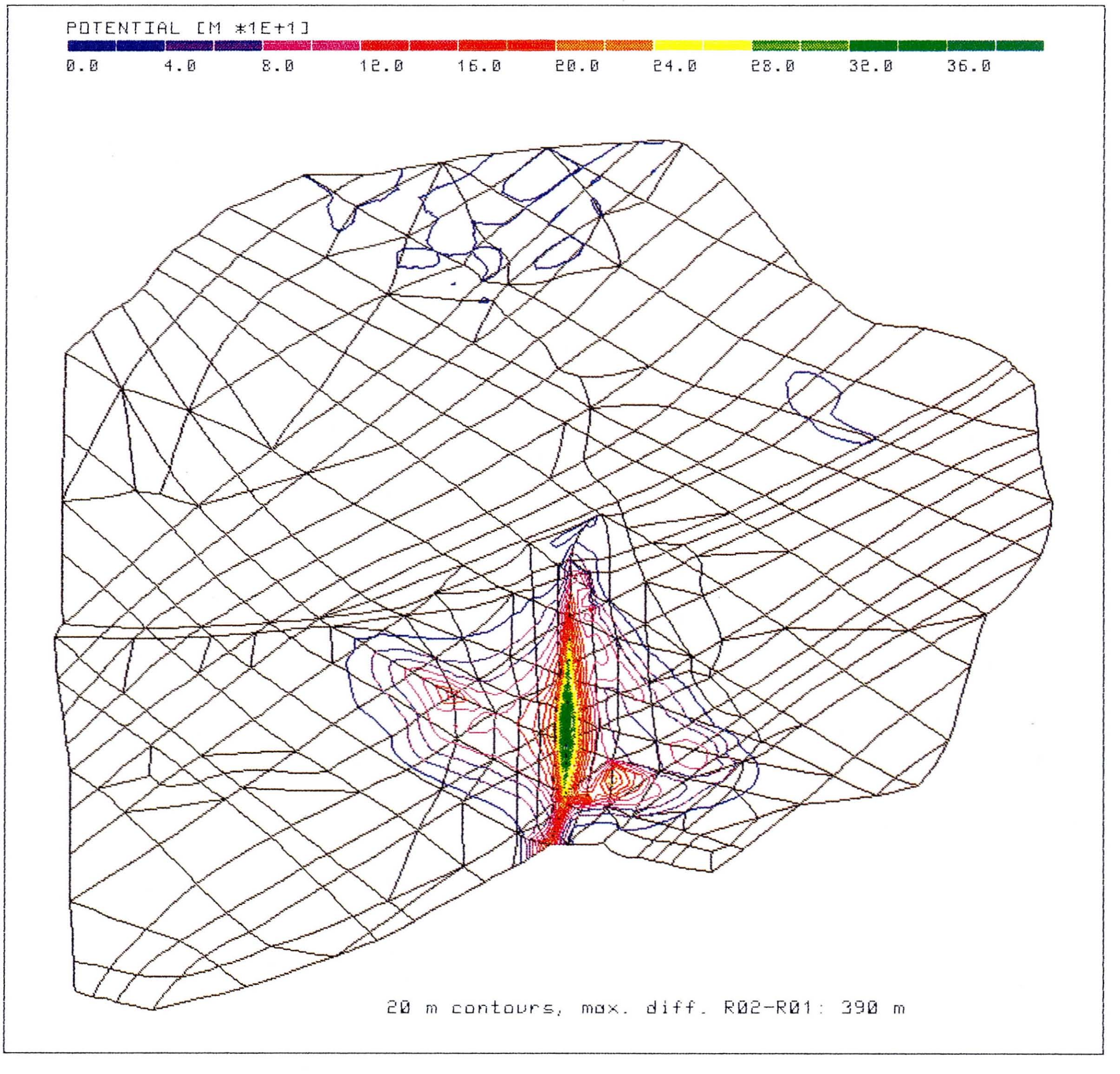


Fig. 13: Calculated head differences R02-R01 on a horizontal section at the GTS level

5.3.4 Significance of the 2-D Fractures

Parameter variations of the water-bearing fracture systems K & S considered the impact on head distribution and water inflows into the tunnel. An increased transmissivity of the fractures (R03) enhances the vertical hydraulic division of the massif and increases the effects of topography. Higher transmissivity results in lower vertical gradients beneath the infiltration and discharge areas respectively. A corresponding reduction of transmissivities in run R04 produces a lower vertical permeability of the jointed massif which reduces the topography effect (steeper vertical gradients). In general, however, the overall impact of these effects on the potential distribution is only of low significance.

More dramatic changes are induced by a restriction of the lateral extent of the fractures. In the run R05 all fractures were hydraulically disconnected along a "barrier" introduced in the third element row adjacent to the main access tunnel on the E and W side respectively. These obstacles interfere with the predominant W-E-oriented groundwater flow within the discontinuities and separate the fractures in the GTS area from their respective infiltration and discharge regions. This effect produces a considerable accumulation of potentials at the upstream side of the barrier (Fig. 14). Despite this lateral screen-off effect, the resulting flux into the tunnel is reduced by only 25 % with respect to the base case. This indicates that the vertical flow from the surface supplies most of the flux into the tunnel.

In the extreme case of R06 all tectonic structures have been desactivated to simulate homogeneous flow conditions as compared with the fractured porous media. The head distribution shows a similar tendency as manifested in run R04 with low-permeable fractures. The effects of topography are further reduced and the inflows into the tunnel are now virtually zero. This is evidence for the groundwater flow within the model being concentrated exclusively in the fracture network.

A specific increase of transmissivities in selected fracture segments was employed in run R09 to reproduce the elevated water discharge into the southern part of the main tunnel. This variation shows only a local impact on the head distribution in the vicinity of Lake Grimsel and has no significance for the remaining model area.

The performed sensitivity study on the water-conducting 2-D fractures can be summarized as follows:

The head distribution and hydraulic gradients in the area of GTS are
- practically insensitive to variations in transmissivity of the fractures
- sensitive to the lateral extent (and thus interconnectedness) of the discrete fractures.

The simulated flux into the main access tunnel is
- directly sensitive to the transmissivity of the discontinuities (proportionality)
- sensitive to the interconnectedness.
- dominated by a vertical flow directly from the surface

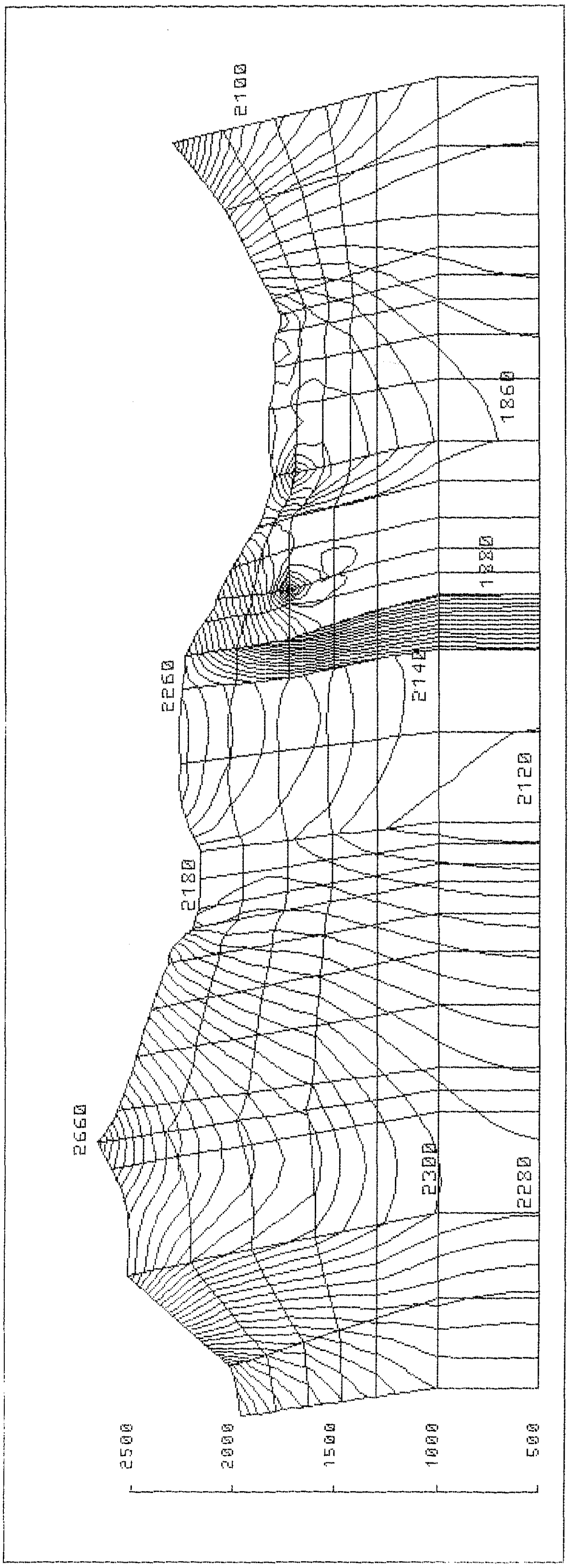


Fig. 14: Run R05: calculated hydraulic heads in vertical section 1

5.3.5 Significance of the BS Zone

As mentioned above, the sensitivity runs covered a wide range of parameter variations due to the virtually unknown hydraulic character of the Bächlisbach zone (BS). This tectonic structure runs from W to E across the model area and intersects both principal systems K and S.

It has been shown that under base case conditions the fault zone exerts a drainage effect on the intersected fractures. By increasing its hydraulic conductivity in run R07, the draining capacity towards the Aar valley is enhanced. At the GTS level the heads in the western part of the BS zone are reduced by 80 m with respect to the base case. In the opposite case of run R08 (with low hydraulic conductivities in the Bächlisbach zone), the fault zone acts as a barrier which intersects most of the water-bearing 2-D fractures. As a result, the northern part of the model is virtually disconnected from the southern part.

In general, the BS feature can be characterized as an important hydraulic heterogeneity within the granitic massif. Its significance, either as a lateral drainage system to the Aar river or as a barrier, depends on the (unknown) large-scale hydraulic conductivity of the disturbed zone. As an important result of the model simulations, it has been shown that this fault zone has no influence on the groundwater regime in the GTS area of investigations.

5.4 Model Calibration

The calibration phase for the regional model aimed more at understanding the general hydraulic behaviour of the modeled granitic massif than at specific calibration of the model results. The available measurements at the scale of the model are very limited. This situation, however, must be considered as characteristic for large-scale (i.e. regional) hydrogeologic models in mountainous, poorly explored areas, so that, in general case, the task of model calibration is likely to be of problematic nature. For the same reason of lacking data, the maximum likelihood approach of calibration, as presented in section 3.3.2, cannot be applied in the case of the regional model GTS.

Generally, the calibration process for a given model extending to the topography surface can include the following data sets:

- measured seepage into underground structures
- observed heads in the drillings
- total surficial infiltration
- travel time + velocity of groundwater (age determination, tracer tests).

In the case of the regional model GTS the calibration procedure used the observed water inflows into the main access tunnel as the primary measure. To compare the calculated with the measured inflow rates the tunnel was divided into three water-bearing sections due to the coarse grid discretization. The sum of the observed and calculated fluxes in each section are shown in Table 6.

MAIN TUNNEL SECTION (m)	Q obs l/min	Q calculated (l/min)					
		R01	R03	R04	R05	R06	R09
700-1000 N of GTS	1.50	1.54	13.13	0.37	1.42	<0.01	1.54
1000-2000 GTS area	3.06	3.36	30.31	0.67	2.80	<0.02	3.37
2000-2314 S of GTS	12.72	2.98	26.88	0.53	1.78	<0.01	12.07
Total Flux	17.28	7.88	70.32	1.57	6.00	<0.04	16.98
% of Q observed	100 %	45%	405%	9 %	34 %	<0.3%	98 %

Table 6: Comparison of observed and calculated fluxes (Q) into the main access tunnel

The base case, which was established as the most probable configuration of parameters, provides a good result for the first two sections. In the southern part, however, neither the number of modeled fractures nor their transmissivity are sufficient to reproduce the elevated fluxes.

The calibration run R09 demonstrates that the available degrees of freedom (here: selective "adjustments" of transmissivity) easily enable an agreement of up to 2 % with the measured total flux to be achieved.

At the scale of the regional model the available head measurments in the drillings from GTS and the main tunnel proved to be of poor suitability for calibration. The grid discretization of the model is too coarse to reproduce the small-scale variation of measured heads. Further, the measurements reflect mostly transient conditions in the vicinity of the tunnel, whereas the model simulates steady-state conditions.

As a rough additional consistency check, the resulting infiltration at the model surface was compared with the yearly precipitation. The modeled infiltrations of 3 m/y at Juchlistock and 2.5 m/y at Gärstenhörner (base case R01) correspond quite exactly to the measured maximum precipitation and are, therefore, too high. This is directly related to the assumption of complete saturation in the model.

5.5 Conclusions Regional Model

Numerical modeling of groundwater at regional scale improves our understanding of the general hydraulic behaviour of the jointed rock mass and of the impact of large-scale anisotropy on the groundwater regime in the vicinity of a repository or rock laboratory site.

Several issues of general validity for any site-specific model were identified at this stage of the regional model.

In the conceptual phase, the complex geometry of tectonic structures requires significant simplifications for modeling purpose. The experience at GTS shows that of the many established discontinuity systems only a few are hydraulically relevant at the regional scale. The latter can be reproduced easily as individual, discrete features in the grid. As a further option, the presence of small structures of hydraulic importance can be simulated by the introduction of a permeability tensor in the rock matrix (anisotropy). The general lack of field data at the regional scale causes difficulties at the stage of mesh layout, since the information acquired from a small-scale observation range (tunnel excavation, drillings) cannot be extrapolated easily to the entire model area.

The relatively coarse discretization of the regional model enhances the effect of the tunnels as sinks. The head distribution reproduced in the model manifests, therefore, a somewhat outsized disturbed zone around the tunnels. The size of the finite elements in the vicinity of underground structures should reach not more than 10 times the size of the elements representing the underground structure in order to simulate the required flow rate within an accuracy of 5 % (KUHLMANN 1987). In the regional model the mean dimensions of the finite elements amount to 200 m by 300 m. Thus it is not surprising that the range of influence of the main access tunnel is that far dominant. This circumstance suggests to take boundary conditions for the local model from the case R02 ("no tunnels") for the initial trial runs and then to subject them to variation in the course of model calibration.

The experience gained during the calibration phase reveals the problematic nature of the calibration process for a regional model in a mountainous, poorly explored area. As a rule, no field data are available for the major part of the model territory. On the other hand, the resolution of the finite element grid is too coarse as to reproduce the small-scale observations resulting from local site investigations.

6 LOCAL MODEL

6.1 Conceptual Model

6.1.1 Model Area and Grid

In contrast to the regional model, the area of the local model is chosen to be as small as possible so as to achieve an optimal relation between the mesh discretization and the number of elements. Since the hydraulic boundary conditions for the local model are taken directly from the regional model, the range of the local model is determined essentially by the extent of the laboratory tunnel and the reach of the exploration boreholes. The dimensions of the local model are thereby fixed at 900 m x 450 m x 400 m. The hydraulically relevant (i.e water bearing) fracture systems S1, S2, S3, K2, and L (KEUSEN et al. 1989), summarized in two principal systems S (S1, S2, S3) and L (K2, K), are modeled as subvertical features analogous to the regional model, but with a higher resolution. Their averaged dip direction and dip angle were defined as follows:

	Dip direction	/	dip angle
$(S_1, S_2) = S$	150°	/	75°
S_3 (locally)	185°	/	80°
(K2, L) = K	210°	/	80°

S_3 is generally considered as part of the S system, however, at some locations it has developed its own orientation, different to the main S direction.

Fig. 15 illustrates the discretization of the shear zones using 2-D elements. In the model the following features are considered:

- shear zones as 2-D elements with individual transmissivities (m^2/s)
- lamprophyres are modeled as 3-D zones, with individual hydraulic conductivities (m/s); the brittle contact of lamprophyres with the country rock is considered as a potential flow path and modeled with 2-D elements
- underground structures, i.e. main access tunnel, laboratory tunnel and caverns, are modeled as 3-D features
- boreholes which furnish useful measurements for model calibration are integrated in the mesh as edges of elements.

Based upon geological observations it has been concluded that the fracture systems S and K play an important role for the water movement through the granitic massif. Therefore the number of hydrogeologic units may be limited to four, distinguishing between granite as rock matrix, lamprophyres and the fracture systems S and K.

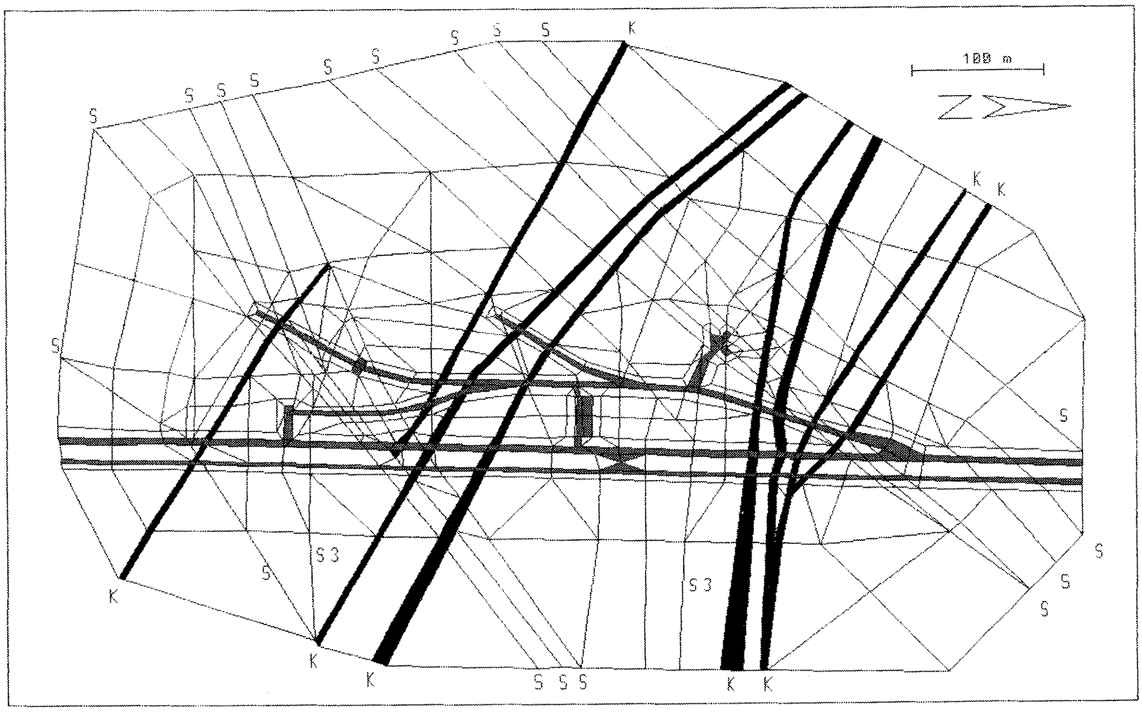


Fig. 15: 2-D mesh of the local model at GTS level: lamprophyres are black, underground structures are grey. K and S indicate the trends of the principal shear zone systems.

The layout of underground structures, which together with the orientation of the geological units constitutes the basic framework of the finite element model, is reproduced by digitizing corresponding blue prints. Since the tunnels are not situated in the horizontal plane but are inclined (GTS tunnels with 1 %, main tunnel with 2.18 %), prescribed isohypses of the tunnel inverts are used to define the z-coordinates of the nodes. For good reproduction of the shear zones the real geometrical direction of these features, especially in the vicinity of the underground structures, is considered. At places where the hydraulic gradient is assumed to be large, a finer discretization is applied (e.g. in the vicinity of structures).

In building the 3-D finite element grid first the 2-D mesh at the GTS level is considered. With a transposition of this mesh along a displacement vector given by the inclinations of the two shear-zone systems S and K and by a prescribed distance of 200 m, two additional meshes are defined and form the upper and the lower boundary of the model. With this procedure the maintenance of small elements is secured, but it is restricted to the case where only two shear-zone systems are modeled and where these are assumed to be quasi parallel. Because of this restriction, the same dip angles were assigned to both the system S3 and the system S.

The 2-D mesh at the GTS level comprises 1'444 elements and 2'327 nodes. The established hydrogeological units and their assumed properties are presented in Table 7 below. The large number of elements is mainly caused by a high resolution in the vicinity of the underground structures. In order to minimize to total number of elements in the 3-D grid, the elements are summarized where a coarse discretization is acceptable, especially in the peripheral area of the model. It can be shown that by using the proposed elimination procedure almost 30 % of the elements and about 35 % of the nodes could be spared. Figure 16 ilustrates this elimination procedure on a selected section.

The 3-D model grid is characterized by the following parameters:

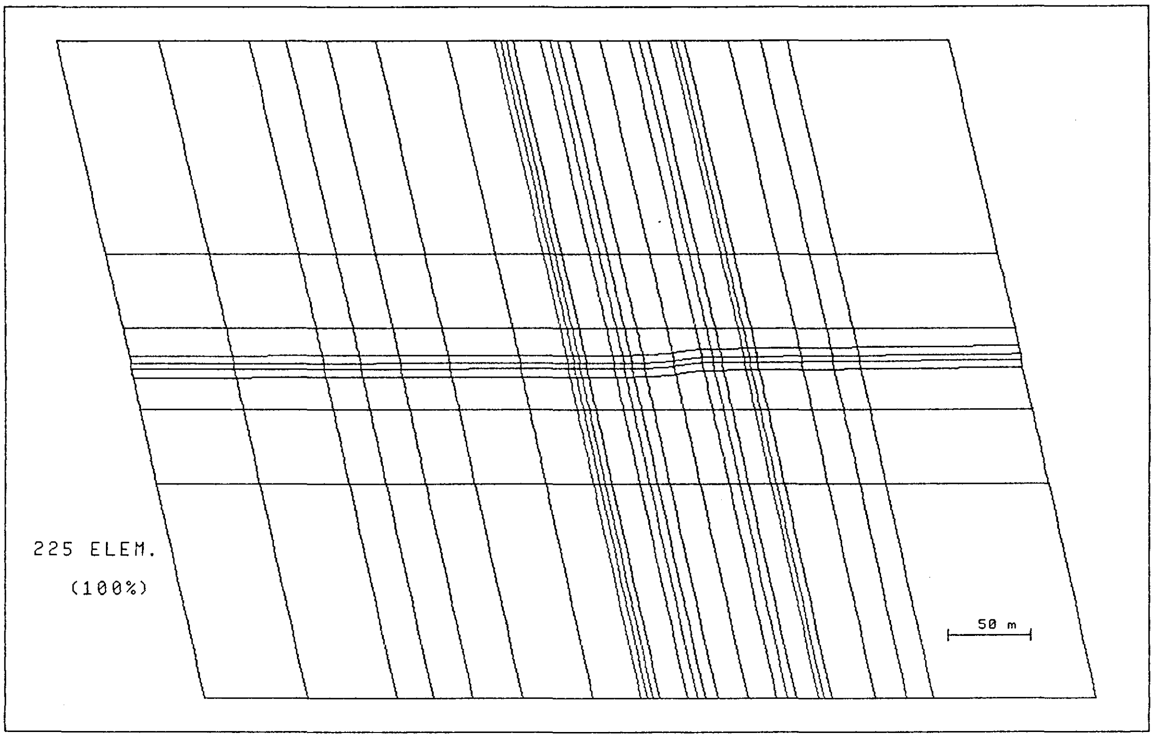
Number of elements:	5'238	3-D
	3'977	2-D
Total	9'215	
Number of nodes:	18'988	
Frontal bandwidth:	676	
Memory space for equations:	101	Mbytes
CPU time (Prime 9955):	18'600 sec (5,2 h)	

6.1.2 Boundary Conditions

At the surface of the model domain fixed hydraulic heads resulting from the simulations of the regional model were used. Though it was initially proposed to take the boundary conditions (i.e. fixed heads) from the model run R02 (without considering tunnels, see chapter 5.3.3), it has turned out during the ongoing simulations with the local model that the reference case R01 of the regional model provides the most suitable boundary conditions, even when reproducing the main access tunnel as an outsized sink.

Because the external boundaries of the local model do not correspond to edges of elements of the regional model, the hydraulic potentials had to be interpolated using the heads at the nodes of the regional model. Due to the regular pattern of vertical shear zones with rather small distances from each other, the head distribution is governed by the properties of the fractures and gives smoothly formed equipotential lines crossing the permeable and the impermeable hydrogeological features. From this point of view the granite massif can be assumed to be homogenous with an anisotropy given by the directions of the principal fracture systems, i.e. in general the hydraulic heads in the matrix are more strongly influenced by the potentials in the adjacent shear zones than by the boundaries. Given the resulting smooth contours of the equipotential lines, the interpolation procedure for the definition of the boundary conditions can be considered reasonable.

The underground structures represent internal boundaries at which the boundary condition h = z is valid (h: hydraulic head, z: altitude).



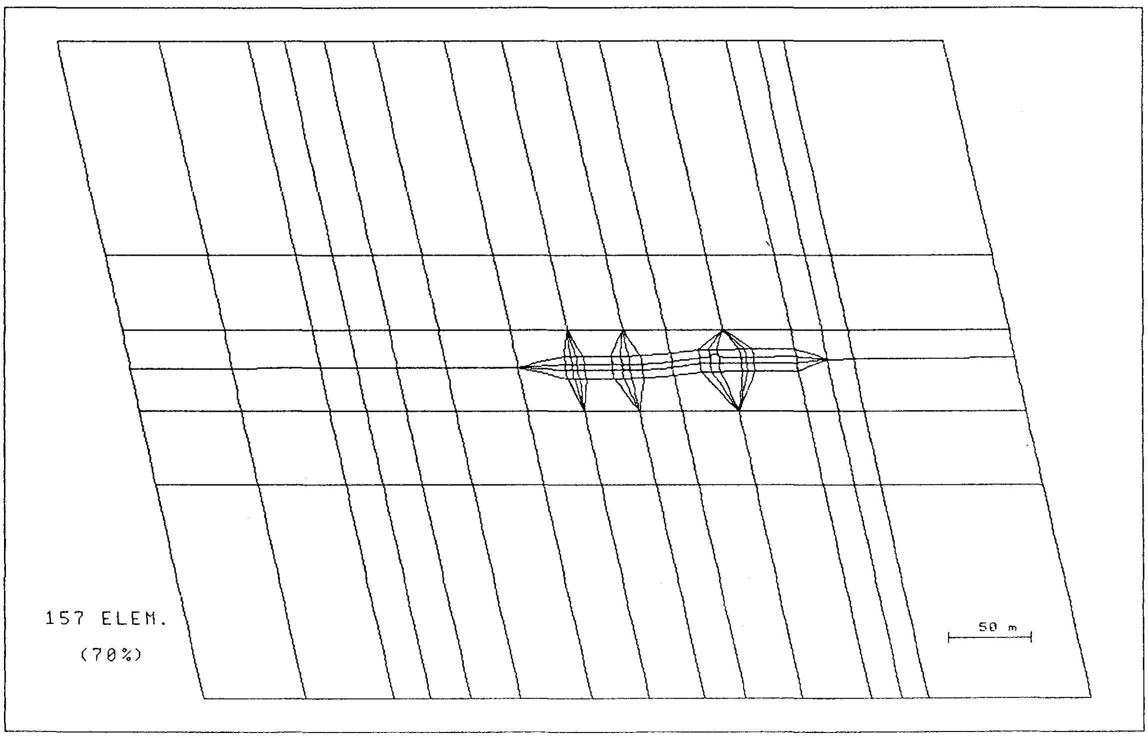


Fig. 16: Effects of the applied element elimination procedure (SHRINK)

6.2 Parameter Variations

Several trial runs with the local model were conducted prior to establishment of the run V05 as the base case. In doing so, a comparison between the calculated and measured total outflow into the GTS tunnel system and main access tunnel was used to provide an approximate check of the suitability of the model input values. As had been proposed in the phase of regional modeling (see Section 5.5), the early runs were performed with boundary conditions obtained from the regional model case R02 considering no tunnels. Due to the excessive fluxes resulting in the model simulation the boundary conditions were then adopted from the reference case R01 of the regional model. Additionally, due to the finer resolution of the local model (i.e. to higher number of discretely reproduced water bearing structures in the model), a reduction of the transmissivity values of the shear zones was required to achieve a further decrease of the total outflow. This inevitable adjustment of the transmissive properties may be explained by the scale effect due to the different sizes of the models. It bears noting that the very coarse discretization of the regional model with only a few water bearing features considered had to be compensated by higher transmissivity of the latter in order to reproduce the observed total flux.

For the simulation of the flow field four different hydrogeological units (permeability classes) were distinguished in the local model. Given the small vertical extension of the model (400 m), a depth-dependent variation of the permeabilities was not considered. The hydrogeological units and their hydraulic properties as established for the base case V05 are shown in Table 7.

K-class No.	Hydrogeological Unit	Dimension of the FE	hydraulic properties
10	Granite matrix	3-D	K = E-11 m/s
20	Lamprophyre	3-D	K = E-10 m/s
30	S-system	2-D	T = E-09 m^2/s
40	K-system	2-D	T = E-08 m^2/s
50	Tunnels	3-D	int. boundary

Table 7: Considered hydrogeological units in the 3-D grid with assigned hydraulic properties in the base case V05

The trial runs described above demonstrated clearly that the parameters which have the greatest influence on the results are the boundary conditions and transmissivities of both shear-zone systems. Therefore, these were taken as the only important input variables for the characterization of the flow field. The parameter variations performed in the scope of model calibration focused hence on the transmissivities of the K- and S-system. Starting from the base case V05 a serie of 8 variation runs (V51-V58) with unchanged boundary conditions was carried out. It is possible to represent all variations graphically by plotting the negative logarithms of both T-values in a XY-diagramm, shown in Fig. 17.

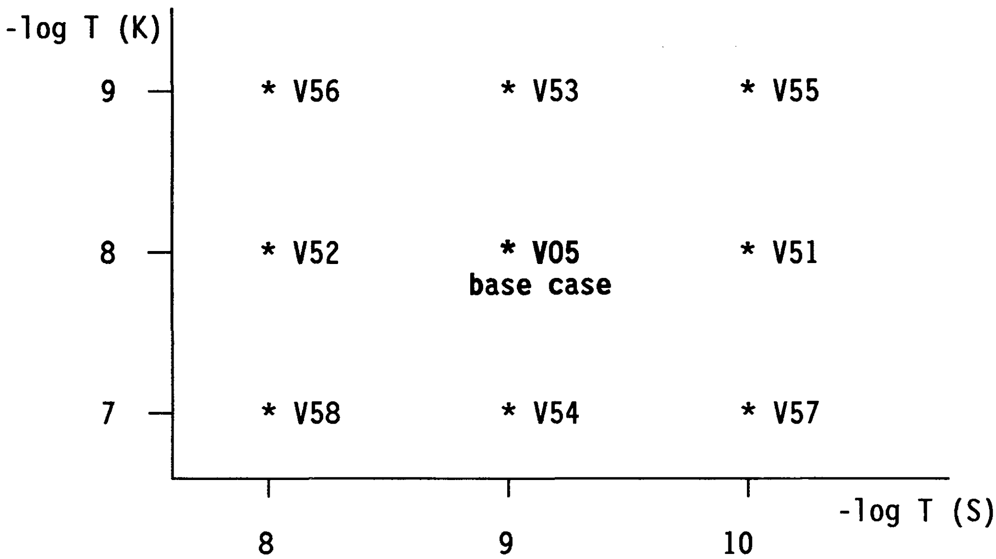


Fig. 17: Variations of the shear zone transmissivities

As a second step, according to the obtained calibration results, adjustment of the boundary conditions was realized in the runs V08 and V09 (see Section 6.3.2). A summary of all performed parameter variations with the local model is given in Table 8.

CASE No.	T (S) [m^2/s]	T (K) [m^2/s]	BOUNDARY COND.
V05	E-09	E-08	R01 (reg.mod.)
V51	E-10	E-08	dito
V52	E-08	E-08	dito
V53	E-09	E-09	dito
V54	E-09	E-07	dito
V55	E-10	E-09	dito
V56	E-08	E-09	dito
V57	E-10	E-07	dito
V58	E-08	E-07	dito
V08	E-09	E-08	reduced by 15%
V09	E-09	4E-08	reduced by 15%

Table 8: Summary of parameter variations in the local model GTS

6.3 Results

The simulation results may be described by the qualitative characterization of the distribution of hydraulic heads on horizontal and vertical sections. The influence of the parameter variations can be demonstrated by showing the differences of heads and fluxes referring to the base case. A more quantitative presentation of the results is possible by selecting a number of flow and head measurements, that are well distributed over the entire model area to give a representative state of the real flow field, and by making use of the proposed objective function presented in Chapter 3.3.2. Since the base case plays an important role for the characterization of the simulation results it deserves a detailed discussion.

6.3.1 Reference Case

The directions of the flow and the corresponding hydraulic gradients at the level of the GTS can be deduced from the simulated horizontal head pattern presented in Fig. 18. The regional groundwater flow is directed from the western part of the model area, which is dominated by the Juchlistock, toward the Aar valley in the East. Due to the Juchlistock massif, the largest hydraulic heads are created at the western boundary of the model. That is why the largest hydraulic gradients are produced at the western side (i.e., upstream) of the underground structures, particularly in the vicinity of the end of the cavern (BK, WT, VE). The head distribution is strongly influenced by the permeable 2-D fractures which limit the drainage effect of the excavations. The largest simulated hydraulic gradient reaches 20(!) m/m and is situated close to the Fracture System Flow Test site BK.

The vertical head distribution in the near field of the underground structures is illustrated by a vertical section crossing the Ventilation Test site (VE) and the Migration Test site (MI, Fig. 19). The cross-section corresponds to the migration shear zone and shows the equipotential contours as concentric lines. The largest hydraulic gradients appear in the vertical direction and reach 3 m/m close to the tunnels. The influence of the 2-D fractures is demonstrated by breaks in the contour lines along the lamprophyres. Hence, the head distribution at the north-eastern side of the lamprophyre is dominated by the heads within the considered 2-D shear zone.

The comparison between the observed and calculated heads in the borehole GS 84.041A, which is a 200 m deep vertical boring drilled from the adit to BK area, is shown in Fig. 20. The imposed boundary condition at the model bottom affect distinctly the reproduced heads in the inferior part of the model. The observed heads are simulated satisfactorily by the case V08, which corresponds to the base case V05 with adjusted boundary conditions (reduced heads). The increase of the transmissivity of the more sensitive fracture system K by half an order of magnitude in case V09 has no effect on the head profile along the borehole.

It has to be emphasized that the measurement sections (packer intervals) in the vicinity of underground structures should be as short as possible to identify clearly the location of the head measurement.

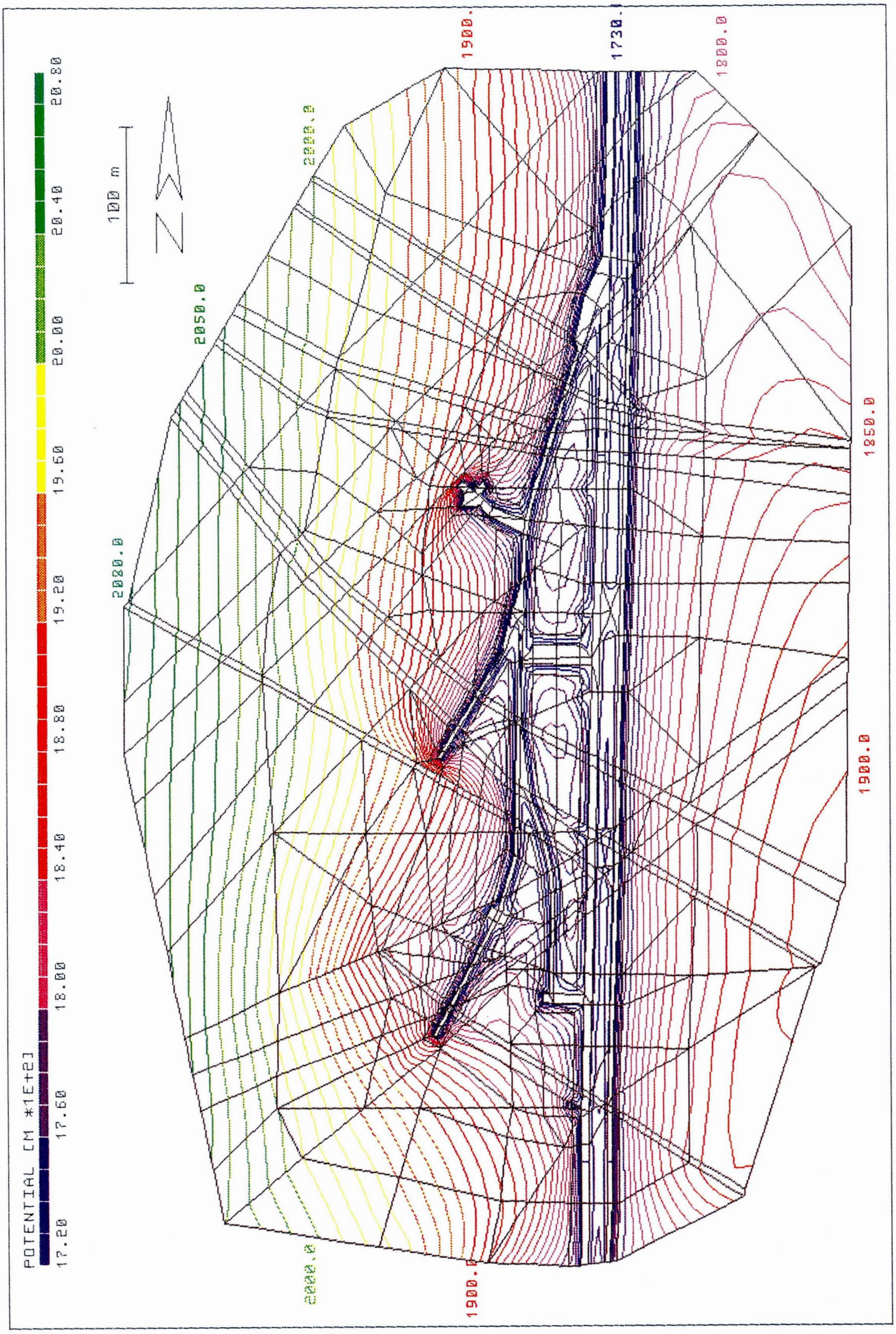


Fig. 18: Head distribution in the base case V05
(horizontal section at GTS level)

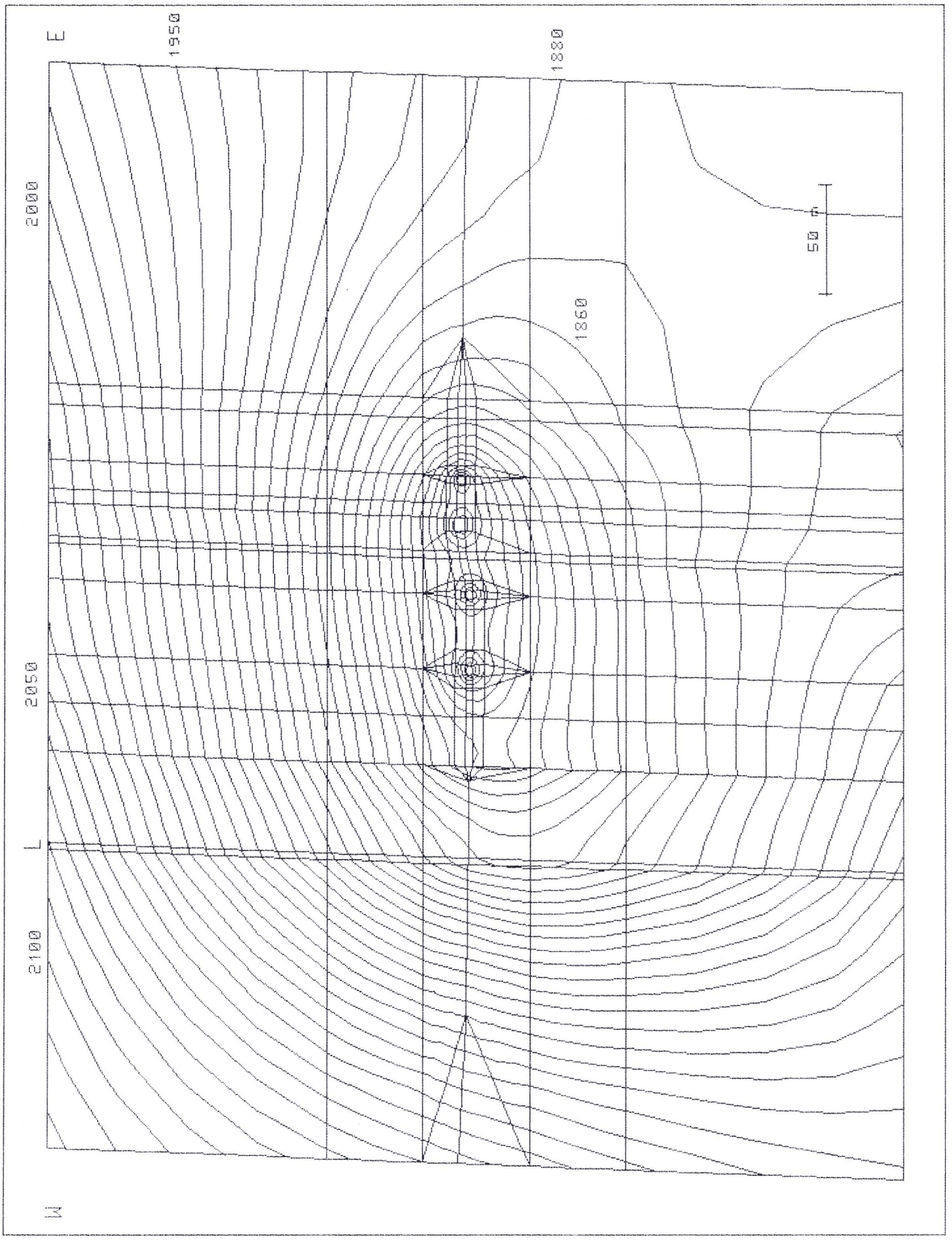


Fig. 19: Head distribution in the base case V05
(vertical section through MI-VE area)

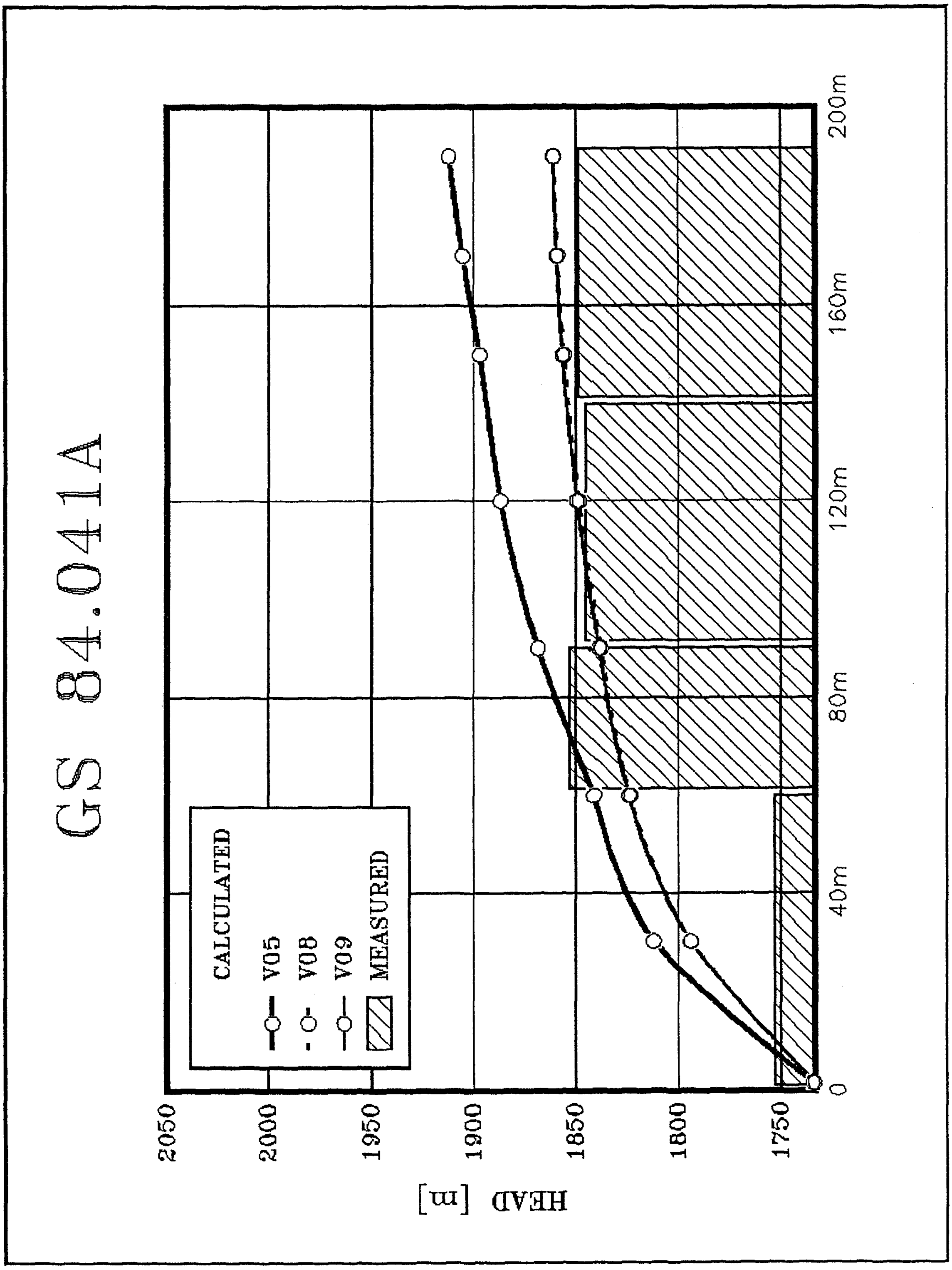


Fig.20: Comparison of observed and calculated head profile along vertical borehole GS (V08 and V09 with identical curves)

Long test intervals have a smearing and averaging effect on the measured head values. The discrepancy between measured and calculated values can also be caused by geometric assumptions (subvertical and quasi-parallel shear zones). The borehole may intersect a given fracture system in the model at a different location than in the reality, particularly at a greater distance from the considered underground structure because of a coarser grid discretization of that area.

To characterize the base case quantitatively, head and flow measurements at different locations are used (see Chapter 4). Table 9 shows the calculated and measured values as well as the estimated errors of measurement. The head readouts represent well-documented selected test intervals in exploration boreholes, whereas the fluxes refer to different tunnel sections as defined in Fig. 7.

No.	CALCULATED IN BASE CASE V05	MEASURED VALUE	ESTIMATED ERROR OF MEASUREMENT	TEST LOCATION
HEADS	m a.s.l.	m a.s.l.	m	
1	1799.0	1816.5	1.8	VE
2	1761.0	1761.7	1.0	VE
3	1778.0	1764.2	1.0	VE
4	1800.0	1752.0	5.0	GS
5	1868.0	1853.0	2.0	GS
6	1889.0	1815.0	5.0	GS
7	1912.0	1849.0	2.0	GS
8	1849.0	1783.2	10.0	BK
9	1884.0	1792.0	10.0	BK
FLUXES	l/min	l/min	l/min	
1	0.40	0.02	0.20	VE
2	0.70	3.50	0.10	WT
3	0.05	2.50	0.10	BK
4	0.20	0.50	0.20	MI
5	1.70	1.80	0.90	remaining section
Q total	3.05	8.30		all GTS

Table 9: Calculated and measured heads and fluxes for the base case

It bears noting that a better match between the observations at discrete locations and the model results could be obtained easily by selective adjustments of transmissivities of the relevant water-bearing structures (K+S) in the corresponding area (i.e., by introducing hydraulically heterogeneous segments of the 2-D systems). However, the calibration efforts were focused on the application and testing of a general calibration method rather than on the reproduction of local observations. Hence, for the description of the general "goodness of fit" of the model, the objective function (1) according to Chapter 3.3.2 is used. Considering the two main terms of this objective function, the base case yields a residual due to head of 1780 and a residual due to fluxes of 1390, both resulting in a total of 3170. A comparison of the total residuals among the calibration runs performed in the sensitivity study (V51-V58, see below) reveals that the base case V05 has the lowest value, i.e. it represents the minimum of the objective function. It should be emphasized that this residual value is strongly dependent on the estimated errors that defined the weights of the measurements. If the difference between the calculated and measured values are of the same order of magnitude as the standard deviation, the square root of J would correspond approximately to the number of measurements. If the square root of J is much larger than the number of measurements either more parameter variations would have to be carried out or the assumptions of the conceptual model would have to be reconsidered.

A closer examination of the differences between calculated and measured heads shows positive values throughout, indicating that the hydraulic potentials at the boundaries were fixed generally too high. It can be envisaged to reduce the prescribed heads at the boundaries in such a manner that the sum of the head residuals reaches a minimum value. However, since the required amount of head reduction at the boundaries is not known a priori, the prescribed heads (taken for example from the base case) should be reduced gradually by a given adjustment factor R and the resulting sum of the head residuals recalculated. Figure 21 shows the anticipated development of the head residual as a function of the pressure adjustment factor R, whereby the minimum is located at the factor 0.85. The basic idea is founded on the assumption that the head within a hydrogeologic unit is more influenced by the potentials at the boundaries than by the prescribed permeabilities or transmissivities. Here linear pressure gradients between the internal and external boundaries are assumed.

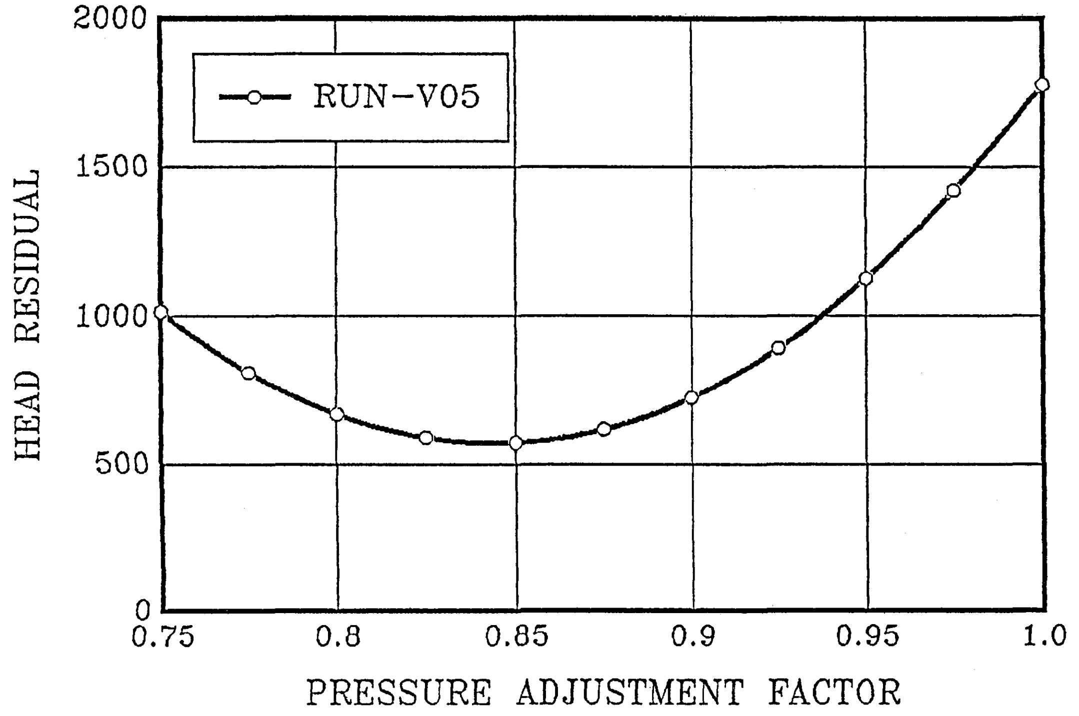


Fig. 21: Variation of the head residuals in response to the adjustment of the water pressure prescribed at the boundaries

In contrast to the heads, the fluxes in a 3-D model depend almost linearly on both the prescribed heads at the boundaries and the permeabilities or transmissivities. A second adjustment factor B is, therefore, introduced in the objective function to vary the flow term. This factor B divided by the first factor R gives the proportional value with which the input value of the permeability has to be multiplied. The **modified objective function J_{mod}** can be written as follows:

$$J_{mod} = \sum \frac{[(h^o - z) \cdot R - (h^* - z)]^2}{(2\sigma_h)^2} + \sum \frac{[Q^o \cdot \frac{B}{R} - Q^*]^2}{(2\sigma_Q)^2} \qquad (2)$$

where z : Altitude of the measurement [m]
R : pressure adjustment factor [-]
B/R : adjustment ratio for K or T respectively [-]
B : flux adjustment factor [-]

The variation of both factors R and B provides a minimum of the total residuals when R is assumed to be 0.85 and B is equal to 4. The ratio B/R gives 4.7 which means that the proposed transmissivities have to be multiplied by a factor of 5.

6.3.2 Sensitivity analysis

The sensitivity of the adopted transmissivity values was investigated by 8 calibration runs V51-V58 (Fig. 17, Tab. 8) that used the same boundary conditions as the base case. For each run the objective function was evaluated. The resulting distribution of the residuals as a function of the transmissivities is presented in Fig. 22. The total residual (a), i.e., the objective function J, shows a local minimum that is situated close to the reference case V05. The same statement is valid for the distribution of the residual due to heads (b). An interesting observation is that in the zone along the diagonal from the bottom left corner to the upper right the variation of the head residual is relatively small. The largest variation is observed along the opposite diagonal. From this it can be deduced that an identical proportional variation of both transmissivities does not essentially influence the head residual. In other words, the head distribution within the model is governed basically by the relative contrasts in transmissivites and of course by the boundary conditions.

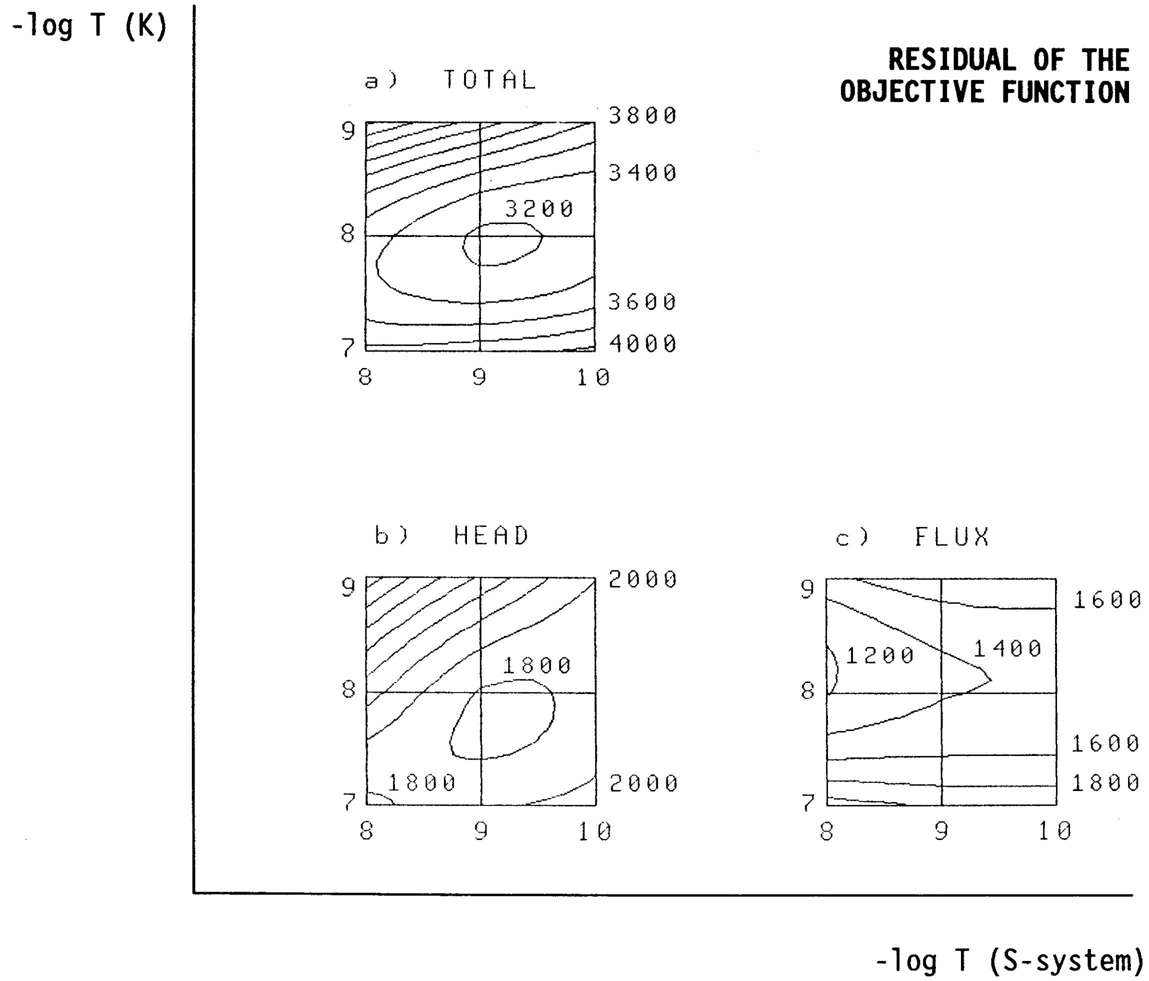


Fig. 22: Distribution of the objective function J (a), head residual J_h (b) and flux residual J_Q (c) as a function of the transmissivities of the S (x-axis) and K system (y-axis)

Variation of the boundary conditions was realized in Run V08. Based on Figure 21 it can be concluded that a reduction of the prescribed water pressure at the boundaries by 15% would produce a significant decrease of the head residual. It is evident that such estimations cannot replace simulation calculations but they give useful indications concerning the correction of parameters and the anticipated reduction of the head residual. In the present case V08, the adjustment of the boundary conditions yields a reduction of the head residuals from 1780 (V05) to 570. Such a procedure is expected to be quite useful in coupling results from models at significantly different scales. The regional model would fulfil its role by providing the reference values from which such an adjustment should start.

The calculation of the flux residual shows a local minimum for the case V52, in which the transmissivity of both fracture systems is 10^{-8} m/s (Fig. 22c). However, for the given values a clear minimum (in the sense of a closed contour) has not been reached, indicating that more variations are needed. The results show that the flux residual is rather insensitive to variations in the transmissivity of the system S, thereby resulting in some uncertainty in the value of this parameter. This is in contrast to the stronger influence of the K system transmissivity. The difference is probably due to the fact that the system K includes a larger number of fractures intersecting the laboratory tunnel than the system S and thus exerts a bigger influence on the flux residuals.

Accordingly, the calculated total outflow (seepage) into the tunnels proves to be more sensitive to the transmissivity of system K than to that of system S. Considering this statement and the fact that a preliminary minimum of the flux residuals has been reached by using the transmissivities of the base case V05 (or V08 respectively), the transmissivity of the "sensitive" system K is changed to $4 \cdot 10^{-8}$ m^2/s (V05: $1 \cdot 10^{-8}$ m^2/s). The recalculation of this run V09 and the determination of the new residuals confirms that this parameter variation provides a better simulation of the measured outflow. The head residual is now about 760 (V05: 1780) and the flux residual is close to 720 (1390) which gives a total residual of 1480 (3170). Thus, in comparison with the base case V05, a reduction of the residual by a factor of 2 has been achieved.

6.4 Conclusions Concerning the Local Model

The simulated groundwater flow through the local model is basically controlled by the adopted transmissivities of the discrete tectonic structures and by the imposed boundary conditions. For the calibration process, hydraulic heads and discrete flux observations within the GTS exploration area were available as primary measurements. Given the sufficiently fine grid resolution in that area and the available degrees of freedom, the simulation results could have been easily fitted to local observations by specific (i.e., location-related) adjustments of the controlling parameter. However, the principal aim of the calibration process was to find a model parameter set which yields the best goodness of fit, expressed by residuals of the objective function.

The calibration method as presented here is based on the identification of a local minimum of head and flux residuals. The limitation of the relevant hydraulic input parameters to three variables (two transmissivities and the hydraulic heads at the model boundary) made it possible to keep the number of parameter variations low and allowed visualization of the results. However, the identification of the absolute minimum of the residuals would require a considerably greater range of parameter variations which could be facilitated by an automatic optimization procedure. The determination of the objective function has shown that the reliability of data measurements plays an important role. It is important, therefore, that all measurements contain a quantitative evaluation of their reliability in the form of a deviation range.

In addition, a practical methodology of adjusting the head values at the boundary, prescribed from a large-scale model with coarser discretization, has been proposed and demonstrated.

7 VALIDATION

7.1 Definition and General Concepts

One of the important objectives of a model building exercise is to develop a tool which allows the behaviour of a known system to be predicted into the future. The degree of confidence with which a model can be used thus becomes a critical factor. This is especially the case in the context of radioactive waste disposal since system performance is typically required to be forecast over tens of thousands of years. Greater attention is therefore focussed on the problem of "validating" a model prior to its application for long-term performance prediction.

Several agencies in the field of nuclear waste disposal have proposed definitions of the term validation and have attempted to outline what might constitute the process of model validation. The U.S. Nuclear Regulatory Commission (NRC) defines validation as (NRC 1983):

> *"assurance that a model (a representation of a process or system) as embodied in a computer code (a set of computer instructions for performing the operation specified in a numerical model) is a correct representation of the process or system for which it is intended"*

The definition of validation according to the International Atomic Energy Agency (IAEA 1982) is:

> *A conceptual model and the computer code derived from it are "validated" when it is confirmed that the conceptual model and the derived computer code provide a good representation of the actual processes occuring in the real system. Validation is thus carried out by comparison of calculations with field observations and experimental measurements.*

The following operational definition of validation has been proposed for the OECD/NEA Stripa project (GNIRK 1990):

> *A model is considered to be validated for use in a given application when the model has been determined by appropriate means to provide a representation of the process or system which is acceptable to an assembled group of knowledgeable experts for purposes of the application.*

In general, then, validation can be thought of as a process to ensure that, for the intended application, the model of interest:

(a) is a physically well-founded representation of the system, i.e., incorporating proper geometrical/geological information, correct physical/chemical processes, etc., and

(b) can predict the behaviour of the system with some acceptable degree of accuracy, as established by comparing model predictions with observations and/or experimental data. These are therefore two key attributes which characterize a validated model.

The representation of a physical system by a mathematical model is a complex, multistage, iterative process involving conceptualization, numerical model formulation, calibration, and validation. The first stage involves establishing a conceptual model which takes into account all relevant geological/geometrical information and appropriate physical/chemical processes. The second stage involves formulating a numerical model that embodies all essential elements of the conceptual model. The next stage is calibration of the numerical model, where estimates of the model parameters (and any associated uncertainty in these estimates) are obtained. The task of validating the model, which is the final stage, should be initiated only after the first three stages outlined above have been completed to satisfaction.

7.2 Validation Methodology

In this section, we propose a general methodology for model validation. The sequential procedure outlined in the following offers a very general set of guidelines that should be useful for validating subsurface flow models as well as other mathematical models describing physical processes.

(1) Identify model capabilities in general, (and intended application, in particular) as well as phenomena and/or observations of interest that can be predicted with some degree of confidence.

(2) Select experimental data (and quantify the uncertainty in the data), or propose suitable experiments to obtain data, for validation such that these are consistent with the capabilities of the model as defined in (1) above. It is also necessary to ensure that this data set complements the data set used for model calibration.

(3) Define quantitative and/or qualitative validation criteria. Quantitative criteria could include goodness-of-validation measures such as the weighted mean square difference between observations and model predictions. Qualitative criteria could involve examining the reproducibility of important features/trends in the data, visually analyzing the degree to which the error bars of the predictions overlap with the measurement error bars, etc.

(4) Generate calibrated model prediction, and also propagate parameter uncertainties to determine the overall uncertainty in the model prediction.

(5) Compare model predictions with experimental data against different validation criteria as defined in (3). Note that evaluation of the various validation criteria, i.e., whether or not they have been "satisfied", is essentially a subjective process. In addition to the modeler's decision in this regard, it is also useful to obtain independent evaluation(s) of the model and its performance at this stage, preferably from a peer group of knowledgeable experts.

(6) If needed, re-conceptualize and re-calibrate; and re-validate, if possible.

The essential elements of the procedure outlined here are also graphically depicted in the flow chart of Figure 23. Note the feedback loops linking the conceptualization and calibration stages to validation. We emphasize again that model building is an iterative exercise requiring continuous updating of the model as more and more information become available.

7.3 Validation of the GTS Local Model

As described previously in this report, a finite element model, referred to as the GTS Local Model, has been constructed to describe saturated groundwater flow in the rock body surrounding the underground rock laboratory at Grimsel. Details of the conceptualization, numerical model formulation, and calibration of this model are presented in Chapter 6. Because of the insufficient amount of in-situ measurements available for model calibration/validation, it was not possible to conduct a validation exercise for the GTS Local Model at this stage. However, it is useful to apply the guidelines for validation suggested in the previous section with specific reference to the GTS Local Model, at least as an example for the application of the proposed methodology.

7.3.1 Model Capabilities

The GTS Local Model is a finite element model capable of simulating steady-state saturated groundwater flow in 3-D. The smallest linear scale represented in this model is ca. 10^1 m, with the largest scale being ca. 10^2 m. At the smaller scale, it is possible to predict both fluxes and potentials with some confidence. However, at the larger scale, the fixed head boundary conditions imposed on the model allow only fluxes to be predicted. Because of the limited spatial scale of

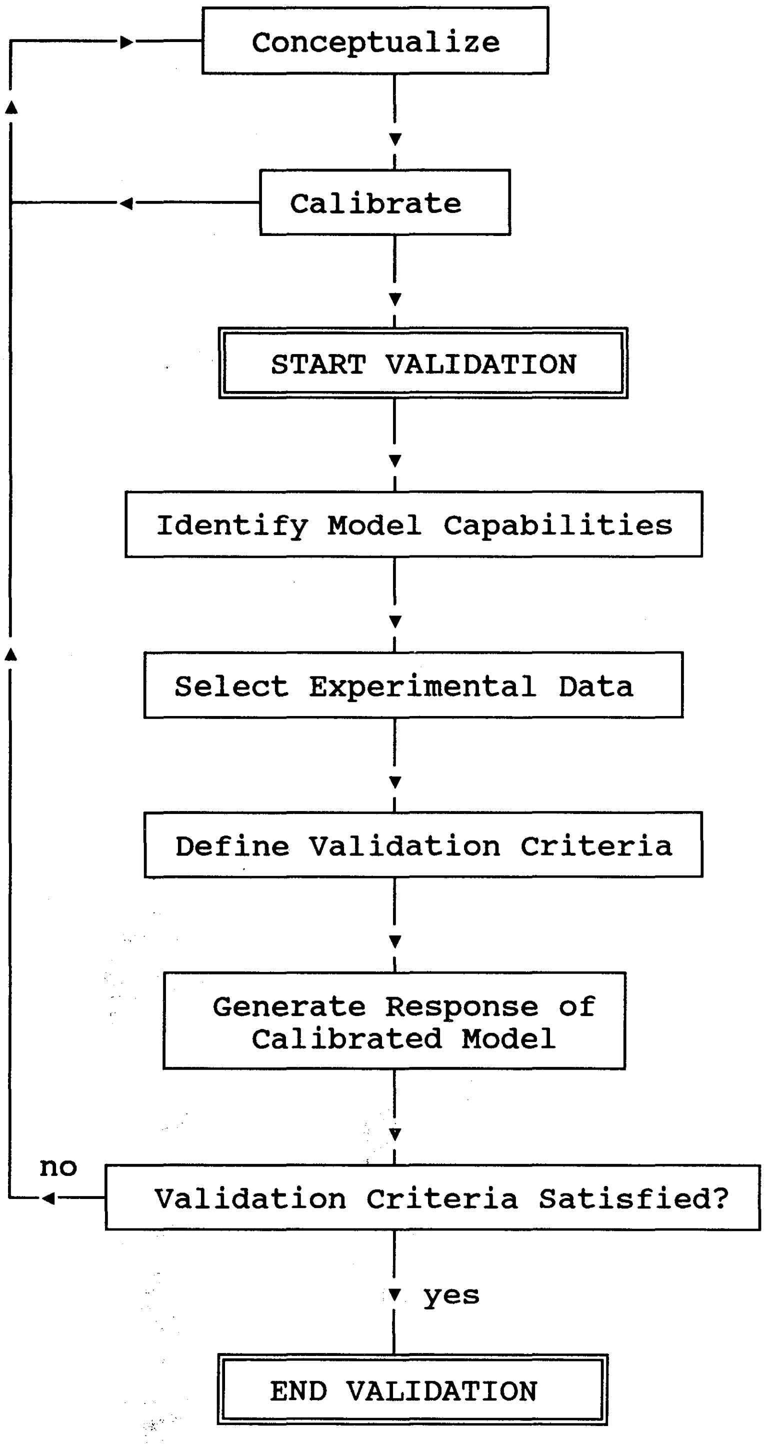


Fig. 23: Flow chart outlining suggested validation procedure

the data used in model calibration, it is believed that flux and head predictions are liable to be more accurate in those areas which provided the calibration data set.

7.3.2 Experimental Data for Validation

Much of the data available from in-situ testing at the Grimsel Test Site has already been used during the calibration of the GTS Local Model. However, there exists the possibility that additional potential data from the Ventilation (VE) test and from hydraulic testing in the deep GS borehole could be used in this process. In addition to the existing data, two other sources for obtaining new information may also be identified. Additional borehole(s) could be drilled in hitherto untested areas to provide estimates of some small and intermediate-scale potential data. The other source of additional information could be measurement of fluxes at old observation points. These could be used to check the reproducibility of the original measurements, and to verify model assumptions relating to zones of high and low flow, regarding steady-state vs. transient conditions, etc.

7.3.3 Validation Criteria

The validation criteria proposed here are based on the recognition that the available measurements are either fluxes or potentials. The fluxes are measured at different points along the tunnel system at GTS, and hence a qualitative validation criteria would be to check zonal flux balances. A similar criterion for potentials, which are generally measured along boreholes, would be to check whether or not the trend of the potential profiles along boreholes is being successfully predicted by the model. For each individual measurement (flux or potential), it is also useful to assign an uncertainty due to measurement/estimation error, and examine how these uncertainties compare with the uncertainty in the model predictions.

A simple global quantitative validation criterion can be proposed based on the **weighted-mean-square difference (WMSD)** between the observed and predicted values, as defined by:

$$J_{val} = \sqrt{\frac{1}{n} \sum_i \left\{ \frac{\alpha_i - \alpha_i^*}{\sigma_{\alpha i}} \right\}^2} \qquad (3)$$

where J_{val} is the WMSD, n is the number of observations, α_i is a generic measurement (flux or potential), α_i* is the corresponding model prediction, and the weighting term $\sigma_{\alpha i}$ is the measurement error. The above equation implies that if J = β, then the average deviation between observed and predicted values is β standard error of measurement. If the measurement error is itself uncertain, then the normalizing term, σ_{ai}, could be replaced by the observed value itself.

7.3.4 Model Predictions Under Uncertainty

The conditions under which the experimental data were obtained (i.e., from static pressure recovery in the borehole intervals following a flow test, etc.) should be used to generate the base case model prediction. The uncertainty in the model predictions could then be obtained via some error analysis procedure. Since the prediction uncertainty is to be used only as a qualitative indicator of validation, it is preferable to use a simple error propagation methodology (e.g., first-order-second-moment analysis) instead of more involved techniques (e.g., Monte-Carlo simulation with Latin Hypercube Sampling).

7.3.5 Evaluation of Validation Criteria

As mentioned before, this critical step in the validation process is also a subjective one. The degree to which agreement between model predictions and observations is deemed acceptable will obviously vary from problem to problem and will also depend on the quality of the observations. In general, however, a minimum criterion should be that the deviations between measurements and predictions be of the same order of magnitude as the measurements. Additional checks should ensure that observed flux balances and trends in local pressure profiles are preserved. The decision as to what is a "reasonable" match and what is an "acceptable" deviation is, of course, a subjective one. In addition to the modeller, it is useful to have other individuals evaluate the model and its performance at this stage - particularly keeping in mind the intended application of the model. If one or more criteria for validation are not satisfied, it might be necessary to modify the conceptual model and/or re-calibrate the original numerical model. The process of validation needs to be re-initiated in this case with another independent set of data.

7.4 Conclusions

Validating a model of a physical system is a complex and, to some extent, a subjective task. Furthermore, the task of validating subsurface flow and transport models in the context of radioactive waste disposal is inherently complicated primarily due to the large time scales involved (ca. 10^{3-4} years) and the uncertainties associated with describing the physical system itself. Validation should therefore be considered in the general framework of model building as one element of an iterative process. As more and more information becomes available about the underground geologic system(s) of interest, the model should be continuously calibrated, validated, and thus, updated. The confidence in the predictive ability of the model, i.e., the degree of validation, is hence a function of time and the amount/quality of information. It is clear that while partial validation of a model according to the above mentioned tenets is possible, "perfect" validation, implying a complete knowledge of the system and its parameters, is a difficult and perhaps an impossible task for models describing subsurface flow processes.

8. CONCLUSIONS AND RECOMMENDATIONS

It has been demonstrated that hybrid hydrogeological modeling, that is, porous medium and small number of discrete 2-D fracture zones, is a useful method for investigating the regional groundwater flow in a fractured rock body under the anisotropic conditions caused by fracture zones. Such modeling also serves to identify domains where special attention is required for the hydrodynamic modeling in the near field of a rock laboratory.

The results show that the relatively large area of the regional model can be discretized in a coarser manner at the model boundaries, to the benefit of the near field of the Test Site, where more information about the flow regime is available. During the second phase of the project a methodology for automatically distinguishing the different resolution requirements of the mesh was developed and applied successfully in the construction of the local model.

Lateral boundaries in the regional model were located at a distance sufficient to reduce the influence of the boundary conditions on the area of the local model. The position of the top boundary is, however, determined by the soil surface, with the usual assumption of fully saturated conditions up to the surface. It should be recognized that high hydraulic heads due to topographic surface elevations have an important influence on the potential distribution even at greater depths, particulary in isotropic media. A variable groundwater table should be also tested, so as to check the influence of the boundary condition at the top surface of the model.

The hydraulic heads calculated with the regional model show only a weak sensitivity to variations of transmissivities or permeabilities and thereby represent a boundary value problem. As a consequence of the regular geometric pattern and the large number of modeled shear zones the hydraulic head distribution appears as approximately homogeneous. In the regional model all shear zones with one exception are modeled as 2-D elements. It seems to be useful to discretize these shear zones with different resolution dependent on their distance from the investigation area (close to the Test Site as 3-D elements and far away as 2-D elements). If the rock matrix is in reality saturated to the surface, the water table in a shear zone need not to be at the same level as in the neighbouring rock but can be much deeper. The 3-D modeling of the shear zones could take account of this circumstance. Another reason for 3-D modeling is the uniqueness of the assignment of the potentials from the regional to the local model. This transfer of the potentials could lead to erroneous interpretation at the intersection of both models. A comparable degree of discretization in both models which would be at least limited to the investigation area and the most relevant hydraulic features is proposed, if feasible numerically.

The calculated hydraulic heads of the regional model correspond to a steady state in which the underground structure would be expected to manifest as an excessive potential sink due to coarse discretization of the grid close to the main access tunnel. Later investigations with the local model show however, that the hydraulic heads taken from the regional model despite this oversized sink are still high. This indicates that the model assumption of full saturation should be varied and if possible verified.

The calculations with the local model focus on the definition of a useful methodology for the construction of the model, with the necessary fine discretization and the exact reproduction of underground structures (by using 3-D elements) and shear zones, as well as on the formulation and application of an appropriate calibration method. For the construction of the model grid, the proposed mesh generation methodology has been succesfully demonstrated. Because of the need for finer discretization close to the exploration tunnels a large number of elements would normally be required. To minimize the total number of elements without reducing the degree of discretization in the nearfield of the underground structures, finite elements of equal hydraulic properties at a certain distance were joined together to form one element. In this way a reduction of 30 % in the number of elements was obtained resulting in significant reductions in computer time and storage requirements.

The formulation of a suitable calibration method is also an important item of the present project. The proposed method shows schematically by a simple example the procedure of identification of a local minimum of head and flux residuals. The visualization of the results of the objective function evaluation helps to judge the sensitivity to the varied parameters. The evaluation of the objective function demonstrates also that the reliability of data measurements plays an important role. It is important therefore, that all measurements considered contain a quantitative evaluation of their reliability in the form of a range of variability.

Furthermore, the water balance in the model region provides a very useful measure enabling adjustment of the calculated flow of each run and thus verification of the plausibility of the input parameters. In general, the total flux in the large-scale range (500 - 1'000 m) can be simulated easily (measured total flux: 8 - 10 l/min; calculated total flux: 8.5 l/min). In the small-scale range (50 - 100 m) a subdivision within the main water bearing fracture systems K and S is necessary in order to reproduce the observed discrete fluxes at the different test locations. This leads to the requirement of more model parameters (e.g., different transmissivities within the VE-drift and BK-zone).

As was also observed for the regional model, the potentials within the local model area are influenced more by the boundary conditions than by the transmissivities. Therefore the calculated heads cannot be varied by sections but have to be adjusted in a global manner by adaption of the boundary conditions. A change of the boundary conditions is justified if a systematic deviation between calculated and measured heads is observed. The investigation of the base case has shown that all differences were positive, indicating that the hydraulic heads at the boundaries were fixed too high. The proposed reduction of the water pressure at the model boundary by 15 % reduces the hydraulic head residuals, J_h, from 1800 to 570 (see Equation (1), p. 11).

With this best estimation of the head field by the local model, suitable and justifiable boundary conditions for a smaller submodel with a high resolution could be performed. This procedure of potential transfer was successfully applied to the submodel of the ventilation test area (JAQUET & THOMPSON 1991).

The comparison between the measured and calculated heads in the GS borehole (GS 84.041A) shows the dominant influence of the prescribed heads at the model boundary while even the influence of the transmissivity of the most sensitive fracture system is negligible. With the proposed reduction of the potentials at the boundaries the measured heads in the GS borehole can be simulated in a highly satisfying manner.

In summary, the modeling exercise completed in the Grimsel Test Site shows that modeling with a limited amount of data has to be performed in an iterative way, checking and updating the various assumptions at each step, until a consistent picture has been reached. Finally, the quality of the results is directly related to the quality of the input data, which have to be compatible with the scale of the model region.

As next steps for further investigation we would propose:

i) to assess the numerical feasibility of providing a comparable degree of discretization for both the regional and local model, at least within the investigation area, in order to facilitate the transfer of hydraulic heads at the model boundaries

ii) to vary the location of the groundwater table as boundary condition and investigate its influence on head and flux distribution within the model

iii) a more in depth analysis of the validation process, if appropriate with an example

iv) consideration of the transient effects, from the excavation (and closure/sealing) of the various tunnels.

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