NUMERICAL MODELLING OF GROUNDWATER FLOW AND RADIOACTIVE WASTE MIGRATION: SELLAFIELD, ENGLAND

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ABSTRACT

Sellafield in NW England was proposed as a candidate site for subsurface disposal in the UK of Intermediate Level radioactive Waste (ILW). Part of the concept of such a site is that the geosphere functions as one of many barriers against serious leakage. Assessment of overall performance requires predictions of the groundwater flow, which may transport radionuclide into shallow aquifers, or to the surface. This thesis develops a 2-D model, which simulate subsurface fluid flow as a means to aid prediction into the far future. The software uses the finite element method, and is an adaptation of OILGEN (Garven 1989). This permits coupling of rock properties, water properties, and flow resulting from differences of potential- including head, density and heat. Mass transport computations are based on a random walk particle tracking model. Data for this thesis was derived from an extensive site investigation program undertaken by UK NIREX.

Conceptually, the regional flow system consists of rainwater falling on 1,000m high ground of the Cumbrian mountains and percolating into the Borrowdale Volcanic Group (BVG), passing westwards by deep flow and returning upwards through the repository site (PRZ), before discharge into overlying sediments and into the Irish Sea. A regional cross section (WSW to ENE) was constructed 115km long and 7.5km deep. This is much longer and deeper than previous studies of hydrogeology in this area. The objective was to reproduce the regional flow and local flow at the repository site. Modelling was carried out progressively, investigating the effects of rock permeability, geometry, anisotropy, faults, salinity and mesh geometry. The approach was to perform a very extensive and prolonged series of sensitivity tests and to adjust each parameter independently to achieve the best fit of predicted groundwater head profiles to head profiles measured in Boreholes 3, 10A and 2. Two sets of best-fit parameters were derived from this calibration exercise.

A second stage of model validation used the two calibrated models to predict the streamlines and residence ages of groundwater in the PRZ. These were compared to the in-situ measured chemistry and salinity of groundwater, and to the measured mean residence age of the groundwater. Only one suite of parameters in the modelling was compatible with both head and residence age measured data. This validated model is taken to be the best representation of the natural regional flow system and to simulate the release of radionuclides from the repository and their pathways towards the surface transported by moving groundwater.

Modelling shows three flow regimes, similar to measured geochemical data: Shallow Flow (high flux); Inland Flow (small flux); Irish Basin (very small flux). Best fit model parameters are close to the median rock permeability measured in the field. BVG permeability is 0.12m/yr and flow rate at the repository site is 1.0m/yr. Recharge is 16km east of the repository. Critical controls on flow are >2km deep permeabilities of Eskdale Granite and Skiddaw Slate, which have not been sampled by boreholes. Water residence age at the repository is predicted as 0.14-0.15Ma by both streamline and dispersion methods; this compares well with measured 0.03-1.5Ma ages. Leachate from the repository reaches the Calder Sandstone 400m deep aquifer after 25,000yr and the Irish Sea bed at 50,000-80,000yr, 3km west of the repository. It is concluded that the geosphere at this PRZ does not greatly assist performance. Previous local models have not correctly considered very deep flow. A PRZ is better sited on the inflow end, not the outflow end, of a regional groundwater system.

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Chapter 1

INTRODUCTION

1 CONTEXT

1.1 Rationale

Following development of the nuclear power and reprocessing industry, the UK government has adopted a policy to dispose of solid intermediate level and some low level radioactive wastes in deep underground repositories. The risk of any nuclear waste returning to the biosphere becomes the main issue in respect of this policy. The problem therefore has both a political aspect and the scientific aspect investigated in this thesis. Sellafield, in West Cumbria (Figure 1.1), is where much of this waste is now stored. Hence this was one of the possible sites being considered for disposal until its rejection in 1996 after a planning inquiry. The long term safety of this site has been examined and debated for years. This research project was initiated when Sellafield was the main identified site, but during the course of this study this status has been thrown into doubt following a public inquiry which resulted in the upholding of refusal to grant planning permission. If the Sellafield site investigation is finally abandoned, the present study will nevertheless prove valuable in terms of lessons learned about how to approach the problem of large-scale hydrogeological simulations. If the Sellafield site investigation is re-opened, the study will have direct relevance.

1.2 Containment

In common with other countries, Britain adopted a “multibarrier” approach to radioactive waste disposal (Billington, 1989). The waste is defined into 3 types: Low, Intermediate, and High level. In Britain this depends on the activity of the waste matrix and so is not directly related to radionuclide content. The waste we are concerned with in this study, ILW, is to be compacted, and placed in concrete within steel barrels. These barrels are placed within a vault below ground and subsequently filled with loose alkaline concrete (grout). These 'near field' features are designed to reduce the solubility of radionuclide chemical complexes. The plan at Sellafield was to place these barrels 650m below ground in low permeability volcanic rocks (Figure 1-2).

The geosphere is one of the barriers of a multibarrier system for the isolation of nuclear waste in a geological repository (Chapman, *et al.* 1987). One reason for disposing of nuclear waste in a deep geological repository is that the geosphere is relatively stable and the geological processes of reaction are much longer than the longevity of human constructions. Thus one would be taking advantage of the stability of the geosphere to provide the long term safety barrier for the nuclear waste. The geosphere also acts as a 'container' to prevent disturbance of the engineered near-field repository. An integral part of the long-term safety assessment of the nuclear waste disposal system is to assess the safety of natural barrier systems. Natural barriers could take the main safety role for the long time periods of disposal required for radioactive nuclear waste. A major feature of safety is controlled by the groundwater flow, through which any escaping radionuclides are transported. Groundwater flow, and associated transfer of radionuclides, is regarded as a major mechanism for transporting radionuclides from a deep radioactive waste repository back to the biosphere. An important aspect of developing a safety assessment for any proposed disposal facility is an understanding of the nature of the groundwater flow. The assessment of these processes requires a detailed understanding of the various physical and chemical phenomena involved. Often the porous material contains several fluid phases, and the various qualities, e.g., mass and heat, can be transported simultaneously throughout the multiphase system. Performance assessment for the disposal of nuclear waste is based on models which predict the releases of radionuclides from the repository site to the geosphere, movement of water and contaminants through the geosphere, the potential risk of radionuclides reaching the biosphere, and impacts on surface life that may occur thousands of years in the future.

A model may be defined as a simplified version of the real (porous medium) system such that the model approximately reproduces the excitation-response of the real system. Efficient numerical methods, advanced computing hardware, and techniques for imaging heterogeneous property distributions, may be combined to examine many of these issues. Assessment of the pollution potential and behavior of constituents in the subsurface requires knowledge of various environmental, geological, and hydrogeological parameters. All of these exhibit large uncertainties due to the practical limits on exploration and investigation, and the natural heterogeneity of underlying geological formations at the waste site. However, there is some recognition that not all commonly used models, simulation strategies, or problem conceptualizations are able to reliably account for all factors that strongly influence radionuclide migration in natural subsurface systems. As heterogeneity exists in the subsurface, restrictive or unjustified assumptions can be made about the state or dimensionality of a physical system, the type of chemical complexing which will occur, or the time and spatial scales that are important. The complexity or uncertainty in physical and chemical behaviour can be produced by heterogeneity in formation materials and their associated properties. Additionally there are constraints on the type and quantity of measurements available to characterise real systems, or oversimplified representations of the fundamental processes present.

Limited knowledge of the variations in fracture density, geometry and conductivity, and of matrix porosities, and the complex groundwater flow field, severely restricts the ability to predict radionuclide migration from subsurface disposal at Sellafield. Although there have been some models created to understand the likely migration of the waste underneath Sellafield, most of them are small scale and consider only superficial systems (Heathcote *et al.* 1996). However, the proposed site is deep underground (over 600m depth) and the fluid flow in the site is inevitably influenced by the deep flow system. The previous numerical modelling of Sellafield was performed by a number of organizations working together (Heathcote et al. 1996), with emphasis on reproducing the groundwater head in the repository site. None of their work was involved in simulating radionuclide transportation. Furthermore, there are some unusual features in this case encountered in the deep groundwater flow system, some of them take very important roles and control the basic flow pattern in this modelling work. For example, saline brine water exists beneath the coastal area, temperature influences the deep flow of groundwater, and the heterogeneity of hydraulic conductivity of rocks and faults are commonly distributed. None of these have been fully answered yet. So, further detailed and large scale modelling is needed to investigate and understand the influence of groundwater on waste disposal for the future.

This study does not attempt to examine the geochemical factors influencing radioactive waste disposal or transport. Neither does it attempt to make a full assessment of safety. The flux rates, and pathways of groundwater flow are investigated in this study. These form a key element of any overall safety case (NIREX, 1995). This study focuses on investigating the roles of salinity, permeability and heterogeneity in controlling groundwater flow in West Cumbria. I have constructed a regional 2D section, 115 km long and 7.5 km deep. Determination of the model parameters is not straight forward, especially in such a regional model where the borehole data are scarce. Data come largely from NIREX reports. NIREX is a company responsible for the geological investigation of Sellafield. From the reports of NIREX (NIREX, 1993) the hydraulic conductivity of the Borrowdale Volcanic rocks hosting a repository at Sellafield has a very big range, from 10^{-3} m/yr to 100 m/yr. So the determination of model parameters is vital in the modelling. Hydraulic conductivity also has scale effects, it seems that large-scale representative values tend to be much larger than those derived from local tests. This effect appears to be more significant for low-permeability media (Carrera, 1993). In recent years, much attention has been addressed towards characterization of spatial variability of field-scale properties because of increasing evidence of its prominent role in field and basin-scale transport (Bosma *et al.* 1993). To understand scale effects in the Sellafield modelling, a smaller scale local section has been extracted and compared with the regional models. It is important that for each model realization the full regional model has been used, even if only the local section has been portrayed in the thesis.

In order to progressively increase understanding of the flow and transport processes in the area and make the modelling as simple as possible, the work proceeded from a simple stage to more complex ones. First of all, reproducing groundwater head is the basis of groundwater modelling work. Emphasis was put on demonstrating the role of regional groundwater flow in directing flow across less permeable basement to focus flow towards the Potential Repository Zone (PRZ) and coastal discharge areas, and on examining temperature and salinity effects. During these model simulations, the data measured in deep boreholes were used to guide the tests. This is to make the simulation rely on the actual natural conditions. Secondly, the chemical composition of the groundwater and likely flow regime is taken into account to help model calibration, building confidence in the model.

Efforts at geochemical evaluation of groundwater are made to analyse the indirect evidence of the site historic evolution and the long term processes that have led to today's conditions; these help to build confidence in the predictions made into the future. This work includes the evaluation of groundwater chemistry and development of models for the origin of different groundwaters. The groundwater is formed, or originates from the precipitation in the recharge area, then flows towards the discharge area. During its movement, there are always chemical reactions between the groundwater, the medium through which the water flows, and chemicals in the water. These reactions can be known by analysing the components and their changes in the water. Some chemistries, such as isotope data, can be used to date groundwater age. A knowledge of solute residence times and groundwater age is important in that it helps to understand the rates of processes within, and times of recharge into, the groundwater system. Eventually the models should provide parameters for the calculation of the consequences of radionuclide transport towards the geosphere.

Despite the wealth of exploration data gathered in the site characterization, the actual volume of rock that is represented by measurements is relatively small. The site characterization is associated with several sources of potential errors and uncertainties regarding equipment, measurement technique, representivity, etc. Many of the parameters used in the site evaluation, e.g. hydraulic conductivity and dispersivity, cannot be directly measured but need to be estimated indirectly using interpretation models. Complex models are frequently derived from the models used to interpret real data measurements. Understanding of these by means of models that aim at realism can provide assurance that the simplifications do not give non-representative results and that field data are used appropriately. The sensitivity test process is built to reduce these uncertainties, assessing both geological and geometrical conditions. However, there is no direct pipeline between site evaluation and the consequence calculation. An important step is therefore to compile results of the site evaluation and model calculations in such a way that different sources of uncertainties can be evaluated. Another important aspect is to ensure consistency between parameters both within a discipline and between disciplines, e.g. between hydrogeology and geochemistry. These allow an identification of the main factors that influence the flow system. During these sensitivity tests, the data measured in-situ under natural conditions were used to guide the tests that rely on the actual natural conditions. The final values of the hydraulic parameters of the rocks differ from those previously reported (NIREX, 1993).

Once a groundwater flow model has been established successfully, with the success of reproducing both groundwater head and groundwater flow regime, identifying those uncertainties, it is possible to make relatively confident predictions through modelling. A mass transportation model was validated using these data. Then a prediction of radioactive waste leaching from the storage site can be made through this model. The final procedure of this modelling is to investigate the pathways of groundwater from the mountain recharge area and radioactive waste movement from the underground storage site through the subsurface system. It is also useful to estimate the safety position by investigating the pathway of groundwater, evaluate the return path and time of the potential nuclide migration from the storage site.

2 OBJECTIVES

The main objective of this study is to characterise and quantify the regional groundwater flow in West Cumbria, focusing on reproducing groundwater head and groundwater flow characteristics measured in situ. This includes testing the applicability of OILGEN transport codes to quantify radionuclide migration in a real flow system; the identification of the relevant transportation processes for consideration in transport models and assessing how successfully those hydraulic and chemical data measured in situ can be reproduced in the models. The goal of performance assessment by means of numerical models is to demonstrate with a high degree of confidence that, in case of a potential release of radionuclides from the repository, the consequences to man and to the environment are below regulatory limits. Groundwater modelling in this thesis is intended to help understand the potential migration of radioactive waste away from the repository zone, and the regional-scale pathway of groundwater flow from mountain recharge area to the coastal discharge area. Modelling also helps to constrain the regional scale geophysical parameters, e.g. by calibrating the model against measured, in-situ data, such as freshwater head and groundwater age. A final objective is to make predictions of radionuclide behavior in situ and assess whether the predictions are controlled by hydrogeology, transport calculations, geochemistry or flow path geometry. These analyses have to be carried out for long time periods. The most important issue is whether numerical safety analyses take into account those migration pathways which may provide the fastest return for the radioactive waste to the biosphere, and result in the highest calculated exposure. The overall aim of modelling is to build numerical models representing the actual behavior of the natural systems, and these objectives are as follows:

- Modelling both local and regional groundwater flow in west Cumbria, to help understand the regional hydrogeological concepts.
- Determination of the regional rock parameters using these models, to quantify both local and regional groundwater flow systems.
- Reproducing the groundwater head in the repository zone, determining the role of the geophysical factors controlling the groundwater flow.
- Identifying characteristics of the groundwater flow field at Sellafield and reproducing the groundwater flow regime by means of modelling, investigating the groundwater flow in faults and fractures.
- Understanding the pathways of groundwater flow which includes tracing the recharge of groundwater in the repository site and its discharge route, the sources of saline water, and dating the groundwater age in the proposed repository area.
- Quantifying the heat transport within the groundwater flow system.

- — Investigating the scale effects upon the hydrogeological parameters and the sensitivity of the geometry in this regional model.
- — Performance assessment of both groundwater flow and chemical component movements in Sellafield.
- — Comparing other workers models, calibrating and validating the models of groundwater flow and mass transport.
- — Assess the long term potential risk of nuclear waste migrating from the potential repository site (PRZ).

3 PREVIOUS WORK ON GROUNDWATER MODELS AT SELLAFIELD

The geological assessment of Sellafield began in 1980 when Sellafield was assessed both for its geological suitability as an existing nuclear-licensed site and for the construction of an underground radioactive waste repository. Since then the geological investigations around Sellafield, West Cumbria were broadly carried out by UK NIREX Ltd. Most of these works concentrated on the local area of Sellafield (20 km x 30 km), around the potential repository, with commissioned new geological, geophysical and hydrogeological investigations. The outer region (60 km x 65 km) was assessed by a commissioned offshore seismic survey. The detail of this work can be seen in a series of reports and publications by NIREX (Chaplow, 1994).

To help understand the potential transportation of radioactive waste by groundwater flow, modelling groundwater flow was performed by a number of organizations working together (Heathcote *et al.* 1996), with emphasis on reproducing the groundwater head in the repository site. Among these, four groups of models were published by NIREX in 1996 (Heathcote *et al.* 1996). They are constructed with differing levels of detail:

1. A two-dimensional areal model which only reproduces the head of shallow wells.

2. Two-dimensional vertical section models (12.5 km long by 2.5 km deep) are simplified and idealised, including some faults that maybe more permeable than surrounding rocks. Groundwater flow was driven by topography, additionally the effect of dense saline fluid was considered.

3. A three-dimensional model corresponded to a cube with sides 5 km long and 1.5 km deep. The results of this model showed that the geological structure as

simplified in the model does not explain the high head seen in Borehole 2.

4. A fracture model incorporated into a volume of BVG 7 km by 5 km, extending to a depth of 1.5 km, comparing the computed pressures at the location of Borehole 2 with measurements, showing the predicted head variability is less than the observed head by about 20m.

From these modelling investigations, the basic concept of topographically driven fresh water flowing west, balanced against saline water from the Irish Sea Basin, flowing rather slowly east, was confirmed (Heathcote *et al.* 1996). However, certain details of the observations remain unexplained. There was no calibration of this modelling. The heads predicted by the model only agree with those in Borehole 3. The model does not explain the observed head in Borehole 2 and the salinity of the eastern source of the saline water. The heads between Borehole 3 and Borehole 2 were not considered in that work.

Haszeldine and McKeown (1995) studied a local hydrogeological model of Sellafield, using NIREX data, and the OILGEN program. They got different results (McKeown and Haszeldine, 1999) from NIREX. The BVG permeabilities deduced were large compared to those reported by NIREX.

Modelling groundwater flow at Sellafield is still at an early stage. There are still a lot of gaps to be filled in explaining the origin of the specific characteristics of groundwater at Sellafield, such as the origins of the salinity of the groundwater, the residence age of it and its flow pathway. The techniques for characterising and modelling fluid flow movement and solute transport through low permeability rocks are less developed than those used for higher permeability water supply aquifers. Although there has been a series of models developed at Sellafield (Heathcote *et al.* 1996), most of them were small scale and mainly used to deal with superficial fresh water flow. Previous work of modelling still remains at the initial level of reproducing groundwater head, no models have been calibrated or validated. They failed to represent the actual deep groundwater flow system where the potential repository site is located. But the proposed site is in the deep underground (over 600m underneath) and fluid flow at the site is inevitably influenced by the very deep flow system.

The issues considered by previous workers

— The groundwater head and flow in the repository zone

— The sources of saline water

— The groundwater pathways
— Calibration and validation of the models

There are some unusual features encountered in the deep groundwater flow system, some of them take very important roles and control the basic flow pattern at Sellafield. For example, brine water exists in the coastal area, temperature influences the deep flow of groundwater, and the heterogeneity and faults are commonly unevenly distributed.

The special features of the hydrogeology in West Cumbria:
— The low permeability rocks
— The deep underground flow system
— The variable salinity distribution from fresh water to brine water
— The faults and fractures prevailing in these rocks

4 LAYOUT OF THESIS

The following chapters present the details of approaching the modelling works undertaken in this thesis. The general regional Geology and Hydrogeology, as well as the relevant necessary geological background of West Cumbria, are introduced in Chapter 2, concentrating on features of the study area of Sellafield. Chapter 3 presents the conceptual model based on the features of geology and hydrogeology in the area. From this conceptual model, the numerical model is constructed. Then Chapter 3 discusses how the numerical model of groundwater flow is created, together with the brief principles of the method, a finite-element method. Chapter 4 presents the progressive development of these models, together with deterministic parameters used in the models, such as permeability, anisotropy, and geometry. As there is still some discrepancy between measured head and values predicted through modelling, the models have to be modified. This is discussed in chapter 5. After all these parameters have been tested and confined in a reasonable range it is confirmed that the computed fresh water head matches the measured head profiles. The mass transport model is constructed in chapter 6, to study the pathway of groundwater using the results of the best fit groundwater flow model. This helps in understanding the potential migration of nuclear waste as well as the water charge from the mountain area to the repository zone. Meanwhile, the groundwater age, known through borehole tests, is also used to validate the model. A final step is to make predictions of radionuclide behaviour in situ and assess whether the prediction is controlled by hydrogeology, transport calculations, geochemistry or flow path geometry. These predictive analyses have to be carried out for long time periods into the future. The most important issue is to take into account migration pathways which may provide the fastest return for the radioactive waste to the biosphere. Lastly, the mechanisms which influence these models, and some new achievements from the modelling are discussed in Chapter 7 and the conclusions are drawn.

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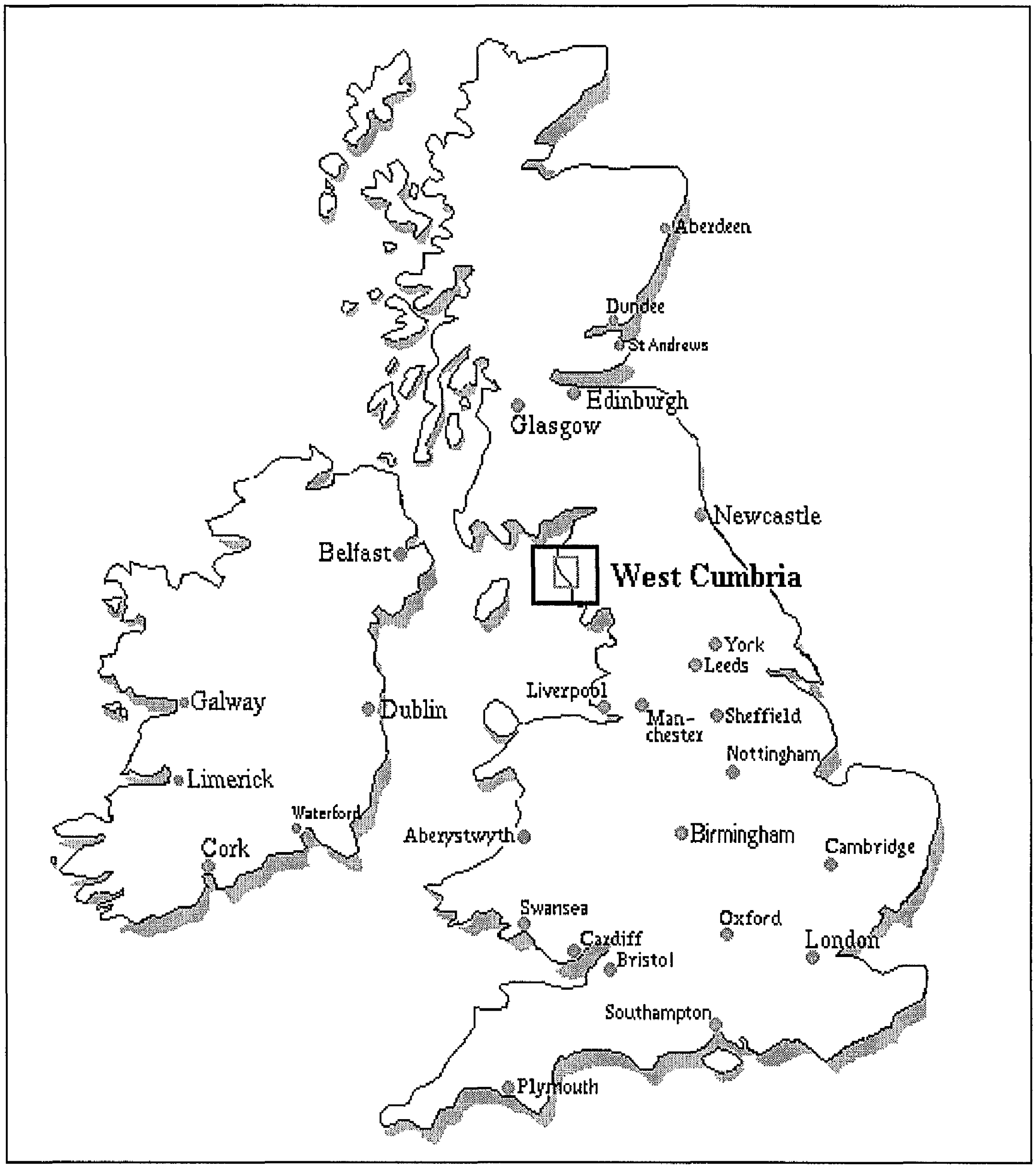

Figure 1-1 Location map of West Cumbria

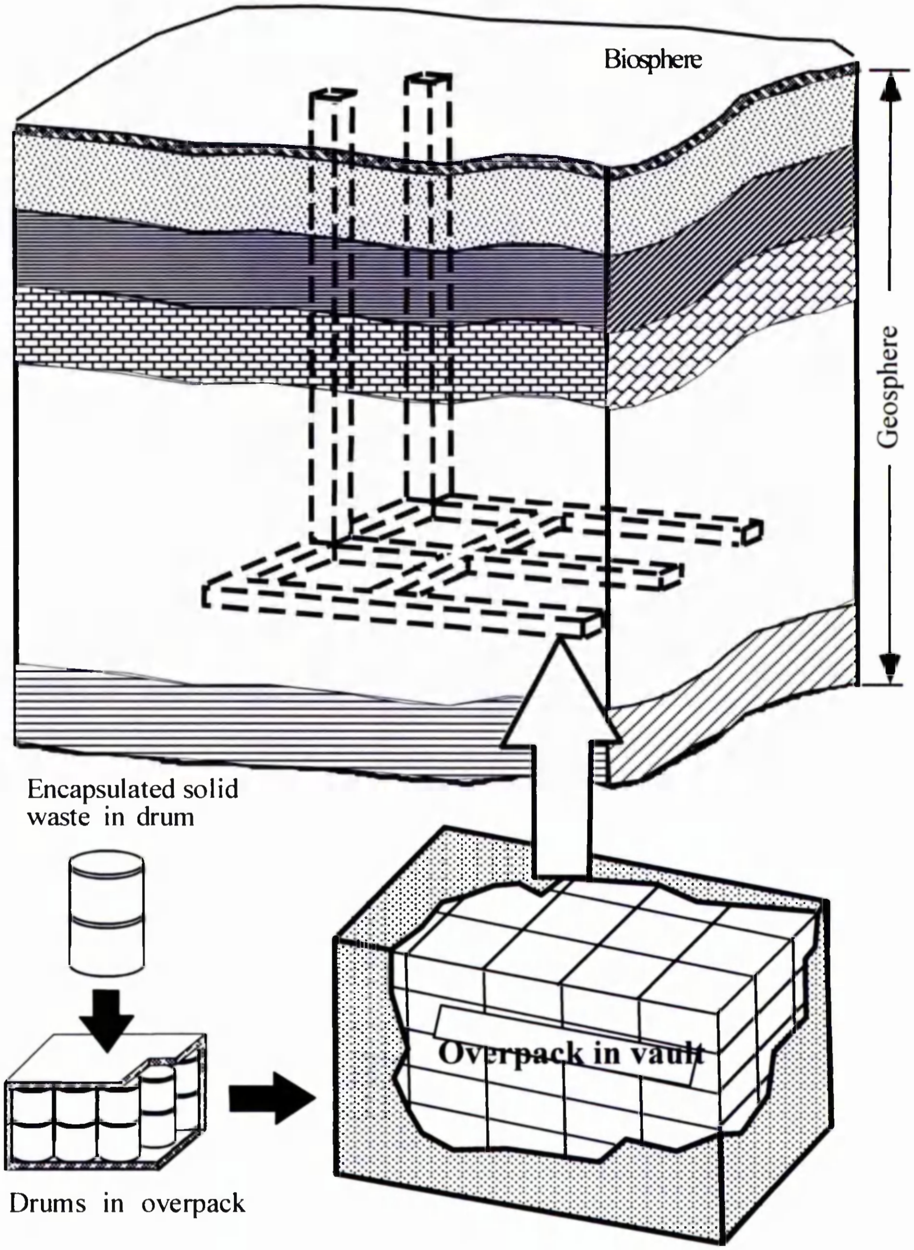

Figure 1-2 The multi-barrier approch to geological disposal

Chapter 2

GEOLOGY AND HYDROGEOLOGY OF WEST CUMBRIA

1 INTRODUCTION

The flow of groundwater, and consequently the mass transport of radionuclides in the subsurface, is an important process by which radioactivity may be carried from an underground waste repository back to the surface. Understanding the groundwater system is dependent on knowledge of the geology. All the geological information used in this study was based on reports by NIREX who were responsible for providing and undertaking geological investigations of Sellafield (Chaplow, 1994). Detailed geological and hydrogeological investigations had been in progress at Sellafield in West Cumbria since 1989 (NIREX, 1993e), including the drilling of 20 deep boreholes. Much of the geological work was at the leading edge internationally and the basic data set is highly reliable (Knill, 1994). This chapter gives a brief description of the geology and hydrogeology of the Sellafield area, providing the information needed for constructing suitable groundwater flow and transportation models. These groundwater models, once calibrated, can be used to make predictions of radionuclide migration in the future, away from the possible underground repository site.

1.1 Location of Study Area

Sellafield in West Cumbria is located in north-west England (Fig 1-1), west of the Lake District. Sellafield lies between the western margin of the Lake District Massif which consists of fractured meta-volcanic rocks, and the adjacent, mainly offshore area of the East Irish Sea Basin. The study area covers a region approximately 120 km east-west by 65 km north-south. The fractured rocks of the Borrowdale Volcanic Group (BVG) of Ordovician age were proposed as the site for an engineered repository for Intermediate Level Waste (Chaplow, 1994). These meta-volcanics stratigraphically overlie the regionally extensive Skiddaw Slate, and are intruded by the late Silurian Ennerdale Granophyre and Eskdale Granite (NIREX, 1992b). Unconformably onlapping the BVG are Carboniferous limestones. These are unconformably overlain by Permian Brockram conglomerate and St. Bees Sandstones, Triassic mudrocks and sandstones of the Sherwood Sandstone Group, and the permeable Calder Sandstone. These Permo-Triassic sediments thicken westwards to the Irish Sea Basin, which is separated from the BVG Lake District by the NW-SE Lake District Boundary Fault.

Quaternary muds, sands and gravels unconformably overlie the sedimentary rocks near the present coastline, and thicken offshore. The geology is summarised by Michie (1994).

2 TECTONIC SETTING

The following is summarised from publications resulting from NIREX investigations (NIREX, 1993a, 1993b, 1993c), and the geological sequence in the Sellafield region is given in Table 2.1. In West Cumbria the present level of erosion is dominated by three westerly-tilted, rhombic half grabens, which closely resemble the tectonic pattern described from the nearby Kish Bank Basin (Jackson *et al,* 1987). The Lake District Boundary Fault is located to the west of present land (Figure 2-1).

The dominant structural features of the area were last modified in the latest Permian and early Triassic (NIREX, 1992b), at which time, tectonism created a system of extensional sedimentary basins. These were defined by major faults, and are parts of a complex system of extensional basins developed on the north-west European shelf (Figure 2-1). The Solway-Carlisle Basin lies to the north of the area, separated from the Lake District Block to the south by the east-north-east trending Maryport and related faults. The East Irish Sea Basin lies to the south-west, bounded to the west by the Lagman and Keys faults. Sellafield lies between the Lake District Block and East Irish Sea Basin.

The early Paleozoic rocks of this area are considered to be "basement". They consist of sedimentary, volcanic and intrusive rocks, associating with the southern margin of the Iapetus Ocean, which closed as a result of the collision between the continental areas of Laurentia and Eastern Avalonia. As a consequence, the early Paleozoic rocks have been subjected to metamorphism (Jackson *et al*, 1987).

In West Cumbria, the oldest rocks, known as the Skiddaw Group (Table 2.1), consist of up to 5000 m of mudstones and intercalated sandstones (NIREX, 1992b). These marine sedimentary rocks of Early Ordovician age were deposited on a continental margin. They commonly exhibit cleavage, and have undergone low grade regional metamorphism and local contact metamorphism. The fundamental, ENE-trending linear, large-scale syn-sedimentary tectonic deformation of the rocks is different from that in the unconformably overlying volcanic rocks. The late Ordovician age Borrowdale Volcanic Group (BVG) consists of a thick (c. 6000 m), dominantly subaerial, basalt-andesite-daciterhyolite volcanic association (Moseley *et al.* 1978). Thickness changes in the BVG are abrupt and controlled by local, syn-depositional volcano-tectonic faulting. However, contemporary faulting and large-scale folding became important in the upper Borrowdale Volcanic Group. The structure of the BVG is dominated by fault block rotations considered to have been produced during caldera collapse (Branney & Soper 1988; Petterson *et al.* 1992). These faults are dominantly vertical and cut through the whole BVG section. Many of the faults now observed in younger sediments were initiated during this phase of caldera subsidence, but persistent northwest or north trends indicate some external control. By the late Ordovician or early Silurian, the volcanic rocks are succeeded, unconformably, by marine, shallow-platform carbonate rocks, the Windermere Group, which are overlain by clastic rocks deposited in a foreland basin. Intruded into these rocks are the Ennerdale Granophyre and the Eskdale Granite components of the late Silurian Lake District batholith (NIREX, 1993b). The Eskdale Granites are composed of two separated bodies, a granite in the north and granodiorite exposed in the southern Lake District.

After a prolonged period of erosion following continental collision in early Devonian times, lithospheric extension and subsidence took place in the Carboniferous (NIREX, 1993b). Carboniferous marine limestones were deposited over the Lake District Massif, with thicker basins in the Irish Sea south and west of the Lake District. The Sellafield area is situated upon the Lake District block, and remained structurally high throughout the extensional episode (NIREX, 1993a). Deposition was relatively uniform as a result of the much-reduced subsidence. From the late Namurian, regional subsidence was sporadically interrupted by episodes of minor faulting and gentle, syn-depositional folding. Towards the end of the Carboniferous, there was regional uplift and erosion, and the Carboniferous rocks were peneplained, weathered and reddened. The effects of the Variscan orogeny within the area were relatively mild, with minor reverse faulting.

Crustal extension was renewed during the Permian. Syn-depositional faulting and half-graben formation caused localised deposition and thickness variations of the Brockram and the Collyhurst Sandstones (NIREX, 1993b). Towards Late Permian time, major normal faulting appears to be absent. The Triassic period began with more-substantial lithospheric extension. The Solway Firth Basin subsided during the Triassic as a sag-basin. The displacement of the Lagman and Keyes faults, and the Lake District Fault Zone, formed an important graben system which is surrounded by the Ogham Platform, Ramsey-Whitehaven Ridge and the Lake

District Block high areas. The overall north trends of the intra-basin faults and the east-trending associated transfer zones indicate that the extensional direction in Triassic times was broadly east-west. The Permo-Triassic rocks lie mainly to the west of the Lake District Boundary Fault. The West Cumbria regional geological cross section is illustrated in Figure 2-2.

3 LITHOLOGIES

3.1 Skiddaw Group

The oldest known rock in this area is the Skiddaw Group (NIREX, 1993b). When exposed to the north of Sellafield, Skiddaw Group rocks consist of mudstones, siltstones and grewackes (see Table 2.1). It is believed that the Skiddaw Group lies beneath much of the Lake District and that it extends under the East Irish Sea Basin to the Isle of Man (Michie, 1996). The group is at least 2 km thick.

3.2 Borrowdale Volcanic Group

In the Lake District, the Borrowdale Volcanic Group comprises a sequence, locally up to 8 km thick, of basaltic, andesitic, dacitic and rhyolitic lavas, sills and pyroclastic rocks along with an abundance of volcaniclastic sedimentary rocks (Millward *et al*, 1994). The BVG thins on a regional scale, to 1500m at Sellafield, and to zero offshore. These rocks are the remnants of a calc-alkaline volcanic field of late Ordovician age. The lithostratigraphy comprises five volcanic formations, consisting of massive tuff, lapilli tuff, or volcaniclastic sandstone, breccia, and clasts, in a sequence at Sellafield of about 1140 m, which is generally subcontinental. The BVG lithologies encountered in all NIREX boreholes are largely the product of explosive subaerial volcanism, probably in an intra-caldera setting (Millward *et al,* 1994). There is a strong lithological control on cleavage development, and well-developed penetrative slaty cleavage commonly exists in the fine-grained volcaniclastic sedimentary rocks.

3.3 Windermere Group

Marine sediments of the Windermere Group unconformably overlie the Borrowdale Volcanic Group and locally the Skiddaw Group (NIREX, 1993a). However, the Windermere Group is absent in the Sellafield area (NIREX, 1993c). This Group is affected by the main deformation of the late Caledonian/Acadian event of end Silurian-early Devonian age (Kneller & Bell 1993). This produced a regional southward tilting, and long wavelength open folds with a NE trending axis.

3.4 Plutonic Rocks

The felsic intrusive rocks at Sellafield are in two main bodies. The Eskdale Intrusion is composed of two separate bodies, a granite in the north and a granodiorite in the south. The Ennerdale Granophyre is dominantly a pink, silica-rich, fine grained granite, 1-2 km thick forming a layered body lying above the Eskdale Intrusion (Evans *et al.* 1993). The exposed parts of the Ennerdale are dominantly granitic and give isotopic ages ranging from late Ordovician to early Devonian (Evans *et al.* 1993). The granite contact is largely concordant with the structure of the overlying Borrowdale Volcanic Group and locally approximates to the base of the volcanic sequence in the study area (Michie 1996). The contact is faulted.

3.5 Carboniferous

There is general a three-fold subdivision of Carboniferous Limestone in Northern England. The Early Carboniferous saw the formation of rifts in which basinal sedimentation were concentrated to the north-west and south of Sellafield. Later general subsidence made the sedimentation spread over a wide area of the Lake District Block including Sellafield (NIREX, 1993c).

Limestone is dominant in the Carboniferous at Sellafield, with subordiary shale and sandstone. The thickness of Carboniferous Limestone is about 200-250 m at Sellafield, thickening to the west towards the East Irish Sea Basin (Michie 1996). These limestones have undergone some degree of diagenesis, resulting in partial or complete obliteration of the primary depositional fabric. Many exposure bedding surfaces are present. Stylolites are abundant and mostly are fine disseminations giving the limestone a pink or pale purplish color mottling.

3.6 Permian

Permian rocks consist of the Brockram Formation, the St. Bees Evaporites Formation and the St. Bees Shale (Table 2.1). The thickness of the Permian Sequence increases westwards, from the Fleming Hall Fault Zone in the Sellafield area, into the East Irish Basin (NIREX, 1993b). At the base of this sequence is a sedimentary breccia known as the Brockram Formation with variable thickness from less than 1m to thicker than 100m. Greater thicknesses, to a maximum of 220m are known in the East Irish Sea Basin (Jackson *et al,* 1987). This unit is coarse, poorly-bedded and poorly-sorted. The evaporites of the St. Bees Formation consist of 50m of carbonate (predominantly dolomite) and sulphates (gypsum/anhydrite) in the Sellafield area (NIREX, 1993c). The St. Bees shales are more extensive into the silty facies above the Brockram over the Repository Zone. The thickness of the St. Bees Shales ranges from 100-200m.

3.7 Triassic and Early Jurassic

Triassic sandstones, known as the Sherwood Sandstones Group, overlap onto the Permian. They are divided into three formations: the dominantly fluvial St. Bees Sandstone at the base, and the overlying, dominantly aeolian, Calder and Ormskirk Sandstones (NIREX, 1993b). The St. Bees Sandstone consists predominantly of pale reddish-brown, very fine to medium-grained sandstone. The Calder Sandstone consists predominantly of dark reddish-brown, fine to coarse-grained sandstone with common, well rounded and frosted aeolian grains. Both are poorly cemented. The thickness of the St. Bees Sandstone and Calder Sandstone is about 600m in total and thickens to 1000m offshore (NIREX, 1993a). The Ormskirk Sandstone is up to 250m thick and developed offshore, although it is not present in the Sellafield area.

The Mercia Mudstone Group that completes the Lower Mesozoic sequence is not preserved onshore, although it is up to 3700m thick in the East Irish Sea Basin (NIREX, 1993b). This group commonly consists of halite and minor amounts of dolomite, dolomitic mudstone and anhydrite.

The porosity in the aeolian facies of the Sherwood Sandstone Group is higher than in rocks of fluvial origin. Much of the porosity is secondary, mainly resulting from dissolution of evaporite cements or detrital grains such as feldspars (NIREX, 1992a).

3.8 Post Early Jurassic, Cretaceous, and Tertiary

After Early Jurassic there was uplift and erosion took place during Cretaceous and Tertiary period, hence there are no sedimentary deposits of these ages in the area (NIREX, 1992b).

3.9 Quaternary

The preserved Quaternary sediments are exclusively the products of the last glaciation (Devensian), and of post-glacial events (NIREX, 1993b). These unconsolidated sediments, with thicknesses ranging from 100m onshore to 200m offshore (NIREX, 1993c), are extremely heterogeneous. They include glacial till, fluvio-glacial gravels, and later deposits of sands, clays, lacustrine clays and peats. There is a broad zone along the coast in which glacio-tectonic effects produced significant faulting and overthrusting within the sequence.

The lithology at Sellafield is summarised in Table 2.1.

4 MINERALIZATION

During the NIREX investigations, mineralogical data have been acquired from detailed core observation, petrographic analysis, fluid inclusion analysis, and stable and radiogenic isotope studies in cores from those deep boreholes. The Lake District has experienced several periods of base metal vein mineralisation affecting the BVG (Firman, 1987). These veins have been worked for galena, sphalerite, baryte and chalcopyrite. Different types of mineralisation and variations in mineral chemistry reflect changes in the type of fluid responsible for the mineralisation, or the evolution in fluid geochemistry.

At Sellafield area a paragenetic sequence of nine temporally discrete 'Mineralisation Episodes', termed ME1 to ME9 (Table 2.2) in order of decreasing age, have been distinguished in fractures (Milodowski, 1995). Many of these are labelled with vein minerals. ME1 to ME3 are hosted only by the BVG and are probably of early Ordovician to Devonian age, and have a high-temperature (150 - 250^{o}C) hydrothermal origin. ME4 to ME7 are correlated with deep burial diagenetic cements found in the Permian breccias and Triassic sandstones. ME7 mineralisation is closely associated with faulting. The study results suggested that ME4 to ME6 should be Permo-Triassic in age, ME7 was initiated in the Triassic and continued into the Tertiary. ME7 is an important episode of hematite mineralisation, possibly of Triassic age. This formed by replacement of Carboniferous Limestone together with veining and oxidation of the BVG (NIREX, 1998). Some 200 million tons of hematite were extracted in the 1800's and 1900's, making this the largest mined deposit in Britain. Both ME8 and ME9 mineralisation clearly post-date ME7 mineral fabrics and are unaffected by the last recognised fault movements. Therefore, ME8 and ME9 are geologically late.

The younger episodes may retain open fractures which permit water flows. These fractures may be filled with calcite, hematite, iron oxides or ore sulphides (NIREX, 1997). ^{14}C data for the calcite indicate that the majority of this ME9 mineralisation formed 40,000 years ago. ME8 mineralisation largely pre-dates this ME9 calcite.

5 HYDROGEOLOGY

An important aspect of the safety assessment of a repository site is to understand the hydrogeology of the site. Therefore extensive hydrogeological work has been done by NIREX to investigate the hydrogeology of Sellafield. Hydrogeological testing and groundwater sample testing have provided additional information on the hydrogeological conditions at the site. The groundwater flow pattern relies on hydrogeological properties on which much of the measurements made come from the testing carried out in the deep boreholes. The hydraulic conductivity of the rocks was initially determined in the boreholes using 50-metre long contiguous section tests. Most of the hydrogeological work undertaken by NIREX was focused on the Sellafield Site (NIREX, 1992e), measuring hydrogeological properties such as heads and conductivities in boreholes. The field borehole tests consist of two categories: tests during drilling and tests post drilling, most of them were carried out in single boreholes without monitoring wells.

5.1 Hydrogeological units and properties

There are two main resources of data on hydrogeological properties, the borehole tests and core characterization (NIREX, 1993d). The hydrogeological properties of the rocks have been derived from field tests and laboratory analysis conducted on core acquired by NIREX deep borehole investigations. Both suites of data may have large ranges of values. Laboratory data can sometimes show less conductivity than field measures, this is due to flow through fractures in situ.

To measure the environmental pressure in the borehole, a drawdown of approximately 50 m was imposed on the test section and then the recovery of the pressure was monitored for 8 or 16 hours (NIREX, 1993d). The pressure was observed on the surface and the hydraulic conductivity can be derived through the 50 m test section (Sutton, 1996). The summarised properties of the rocks are shown in Table 2.3. The hydraulic conductivity obtained from the test in each lithology can be summarised as follows:

5.1.1 *Calder Sandstone*

Hydraulic conductivity estimates in the Calder Sandstone (measured by gas) calculated for core samples range over 3.5 orders of magnitude (NIREX, 1993d). The median value of horizontal hydraulic conductivity is 4.8×10^{-7} ms^{-1} and the median value for vertical hydraulic conductivity is 2.1×10^{-7} ms^{-1}, which suggests that the intergranular conductivity is anisotropic with a slightly higher horizontal conductivity. The field hydraulic conductivity estimates range over 2.7 orders of magnitude with the mean value at 1×10^{-7} ms^{-1}. The porosity estimates range from 13.4% to 26.3% with the mean at 19.5%.

5.1.2 *St. Bees Sandstone*

Hydraulic conductivity estimates from core samples in the St. Bees Sandstone (measured by gas) range over 5 orders of magnitude (NIREX, 1993d). The median value for horizontal conductivity is 2×10^{-8} ms^{-1} and the median value for vertical core hydraulic conductivity is 5×10^{-8} ms^{-1}. From this it is inferred that the intergranular conductivity is anisotropic with a ratio of 0.4 and the higher permeability is perpendicular to the bedding. The field hydraulic conductivity estimates range over 2.7 orders of magnitude with the mean value at 3×10^{-8} ms^{-1}. The porosity estimates range from 1.5% to 21.6% with the mean at 11.6%.

5.1.3 *St. Bees Shale*

The horizontal core hydraulic conductivity estimates (measured by gas) range over 2.9 orders of magnitude (NIREX, 1993d), with the median value 8×10^{-8} ms^{-1}. The vertical hydraulic conductivity ranges over 2.3 orders of magnitude, with the median value of the hydraulic conductivity at 3×10^{-11} ms^{-1}. In contrast, the field hydraulic conductivity estimates range over 4 orders of magnitude with the mean value at 2×10^{-9} ms^{-1}. The porosity estimates range from 13.4% to 26.3% with the mean at 19.5%.

5.1.4 *St. Bees Evaporite*

The core hydraulic conductivity estimates in the St. Bees Evaporite (measured by gas) range over 3 orders of magnitude with the median value of 7×10^{-11} ms^{-1} (NIREX, 1993d). The horizontal and vertical core hydraulic conductivity are similar. The porosity estimates range from 1% to 14.1% with the median at 11.6%.

5.1.5 *Brockram*

The core hydraulic conductivity estimates (measured by gas) range over 3 orders of magnitude with a median value at 4×10^{-10} ms^{-1} (NIREX, 1993d). The field hydraulic conductivity estimates range over 6 orders of magnitude with the median value at 6×10^{-10} ms^{-1}. The porosity estimates range from 0.6% to 11.4% with the median at 4.2%.

5.1.6 *Carboniferous Limestone*

The core hydraulic conductivity estimates (measured by gas) range over 2.2 orders of magnitude, with a median value at 3×10^{-11} ms^{-1} (NIREX, 1993d). In contrast, the field hydraulic conductivity estimates range over 3.5 orders of magnitude with a median value at 5×10^{-8} ms^{-1}. This is much higher than that of core test and indicates that the flow within the Carboniferous Limestone is dominated by the presence of fractures. The horizontal and vertical core hydraulic conductivity estimates are similar. The core porosity estimates range from 0.2% to 5.9% with the median at 1.2%.

5.1.7 *Borrowdale Volcanic Group*

BVG is fractured at all scales, and most of the fractures are healed or infilled (sealed) but a subset are at least partially open and provide pathways for groundwater flow (NIREX, 1993d).

The core hydraulic conductivity estimates (measured by gas) range over 6 orders of magnitude, with a median value at 4×10^{-11} ms^{-1} (NIREX, 1993d). The field hydraulic conductivity estimates range over 7 orders of magnitude with the median value at 1×10^{-10} ms^{-1}. No significant difference is measured between the horizontal and vertical core hydraulic conductivity estimates. The porosity estimates range from 0.1% to 7.2% with the median at 0.8%. The voids in the BVG consist of microfractures.

5.2 Hydrogeochemistry

Hydrogeochemical data indicate the origins of groundwaters, and may help in tracing past movements and constraining the residence times. Some aspects of groundwater chemistry (e.g. salinity) also control the groundwater flow pattern and solute transportation, and may affect radionuclide migration. The following discussion focuses on the salinity distribution in the area, because salinity has a direct impact on groundwater movement. The water components have been measured in laboratory data from samples collected and screened to eliminate contamination by drilling fluids (NIREX, 1993d).

5.2.1 *Chemical Compositions*

The variation of salinity was observed and calculated from the total dissolved solid values for the groundwater samples or on the basis of electrical conductivity data. Groundwater conductivity increases steadily from less than 100 μS/cm in the eastern area underlain by the BVG to more than 400 μS/cm adjacent to the coast. The regional alkalinity also increases away from the BVG towards the coast.

The chemistry of shallow groundwater results from rainfall, anthropogenic inputs, interaction with aquifer minerals, and mixing with deeper water sources. The chloride concentrations of shallow waters generally reflect rainfall and fertiliser inputs. Deeper waters have a large number of samples which could contain contributions from the two other obvious sources: sea water and deep saline water. These two are distinguished by their Na/Cl and Br/Cl ratios. Deep saline water is inferred from one record of saline water in the base of a lake (NIREX, 1993d). The realistic upper limit for deep saline groundwater to contribute to the near surface groundwater might be 3%.

The compositions of deeper groundwater are separated into Na-Cl dominated saline waters at depth and shallow Ca-HCO_3 dominated dilute waters (NIREX, 1993d).

5.2.2 *Salinity Variations*

Groundwater at depth in Sellafield is saline (Bath *et al*, 1996). The salinity of groundwater is obtained from information on groundwater density. The density of groundwater is determined by its salinity and temperature. The in-situ salinity was calculated from electrical conductivity data and chemical analysis of groundwater samples. Regionally, 4 salinity types are inferred: (1) A very saline dense brine (>100 mg/l) beneath the Irish Sea, derived from long periods of rock-water interaction with evaporites. (2) A fresh water (<10 mg/l) in the actively flowing shallow aquifer of the Calder Sandstone. (3) A deep saline water (10 - 100 mg/l) inferred from saline water collected at the basement of rocks in which the groundwater flows through resulting in water-rock reaction. The origins of this salinity are obscure, but may relate to water interaction with minerals, the detail of this discussion will be addressed in chapter 6. (4) A surface cap of meteoric rainwater below the Lake District.

The contours (Figure 2-4) for groundwater density show the position of the saline interface. In Boreholes 2 and 10A, the interface occurs at 320 m below the Ordnance datum (bOD) and 680 m bOD respectively, which appears to correspond with the geological boundaries of the base of St Bees Sandstone. In Borehole 3, the interface is at 559 m bOD between the Calder Sandstone and St Bees Sandstone (NIREX, 1993d).

Beneath the saline interface, the salinity varies greatly from borehole to borehole. The salinities at depth are high in Borehole 3 and Borehole 10A, and a maximum of 108,000 mg/l Cl is recorded in Borehole 3. The salinity at 650 m bOD depth within the Potential Repository Zone and Borehole 2 is lower than that in Boreholes 3 and Borehole 10, with maximum recorded value of 17,000 mg/l Cl. Surprisingly, the salinity of groundwater in the Carboniferous Limestone in borehole 3 has a somewhat lower value than the overlying and underlying groundwater, which is explained later in Chapter 5.

5.2.3 *Origins of saline waters and brines*

The Br/Cl ratios for saline groundwaters and brines in Boreholes 2 and 3 are relatively uniform with depth even across the lithological boundaries. The ratio of Br/Cl in Borehole 2 is higher than in Borehole 3. The variation of the ratio suggests that there might be two sources of salinity: one which dominates in Borehole 3 and the other one with higher Br/Cl ratio in Borehole 2. Groundwaters in Borehole 3 have a constant Na/Cl ratio (ca 0.66 by mass) with increasing salinity whereas saline BVG waters from Borehole 2 show a trend of decrease. This trend in BVG water is interpreted as a result of progressive water-rock reaction in the BVG which depletes Na (NIREX, 1993d).

There are some conclusions by NIREX from the comparisons of Cl, Br, Na, SO4: (NIREX, 1993d)
—One salinity source is the basinal fluids offshore to the west
—another source is tentatively thought to be the BVG basement in the east
—brines and saline groundwaters originate from meteoric water recharge
—saline waters in the PRZ are isotopically distinct from shallow groundwaters

—Basinal waters have a distinctive evolution with an isotopically heavy end member brine

—similarity between saline groundwaters and fluid inclusions in BVG veins suggests that these groundwater conditions have persisted over a geologically significant period of time.

5.2.4 *Isotopic Compositions and Groundwater Age*

Stable isotopes (δ^2 H and $\delta^{18}O$) for groundwater samples indirectly suggest that the age of groundwater in the BVG of the PRZ is between 10,000 and 1,500,000 years (NIREX, 1993d). This is because the stable isotope ratios are light, and suggest recharge was cool and reflected pre-glacial conditions. The samples taken from Borehole 2 have a meteoric signature that is lighter than that of present day rainfall. Noble gas recharge temperatures also indicate that recharge conditions for groundwaters in the BVG of the PRZ were colder than that in the sandstones. All these indicate that the recharge of basement rocks in PRZ was under colder climatic conditions possibly within the last glacial period (Pleistocene) that commenced about 1.6 Ma and ended 10,000 years ago. The interpretation of data on carbon-14, helium-4 and the ratio of chlorine-36 to chloride leads to similar conclusions. The absence of ^{14}C from BVG samples suggests that the groundwater is in excess of 30,000 years old. The $^{36}Cl/Cl$ ratios measured in saline waters in Borehole 10A lead to the conclusion that mixing has taken place more recently than 1.5 Ma ago (NIREX, 1997). The signature of groundwater in the basement rocks of the Potential Repository Zone range from 22 to 28×10^{15}, to reach this equilibrium most of the chloride in the groundwater in the BVG has been isolated from the ground for around five half-lives (1.5 Ma).

The stable isotopic signatures in the brines at Sellafield are heavier than those elsewhere in the region which might imply recharge prior to the last glacial epoch (NIREX, 1997). In Borehole 10A and within the St. Bees sandstone to the west of the site on the base of the coastal plain regime, the isotopic values are also lighter and these indicate an older and cooler recharge.

5.3 Regional hydrogeology

5.3.1 *Hydrology*

The climate varies from high relief inland with rainfall within 1500-3500 mm/yr to the low relief coast with rainfall around 965-1015 mm/yr (NIREX, 1993d). The physiographic divisions of the region are the Cumbria Mountains and a coastal plain. The coastal plain rises steadily to the north east from around 20 m above Ordnance datum (aOD) near the coast to around 100 m aOD inland. Further north-east inland, the topography rises more steeply and forms the hills over 300 m high, with summit elevations up to 978 m aOD. The river Bleng joins the river Irt in the south and, together with the River Mite and the River Esk, forms an inland extension of the coastal plain at the entrance to Wasdale (NIREX, 1993d).

5.3.2 *Distribution of Groundwater Heads*

The groundwater heads are calculated from Environmental Pressure Measurement (EPM) tests undertaken by NIREX (Sutton, 1996). The distribution of groundwater heads illustrates the groundwater flow potential and the potential gradient, these are presented in Fig 2-4.

The fresh water head contours show a gradient from the higher ground in the east towards the coast in the west. The horizontal gradient decreases to the west. Small vertical gradients are also present through most of the fresh water region. The heads have a stepped increase across the top of Brockram. Such features have been assumed to exist throughout the Brockram, indicating that the Brockram has low permeability features that confine the underlying high heads.

There is little head gradient to drive groundwater flow through the interface of saline water. The groundwater topographically beneath 1025 kg/m^3 density contour is likely to be almost static (NIREX, 1993d).

5.3.3 *Groundwater Flow Systems*

From NIREX hydrogeological investigations of hydraulic head and geochemistry, the groundwater flow system can be divided into three regimes (Figure 2-5): Coastal Plain Fresh Water Regime within a superficial aquifer system, the Irish Sea Basin Brine Water Regime in the west and the Basement Saline Water Regime.

Groundwater flow within the shallow Sherwood Sandstone Group and the eastern top BVG is fresh water and driven by gravity. It has a large horizontal component because of relatively high hydraulic conductivity. From the map of the groundwater table, the overall groundwater flow is from hills Northeast towards the coast Southwest (NIREX, 1993d).

The brine waters in the west are interpreted as being derived from dissolution of evaporites and as associated with Irish Sea basinal processes. These dense saline groundwaters are inferred to be static, and have been tested in the vicinity of Boreholes 3 and 10A. (NIREX, 1993d)

The saline waters within the deeper BVG may be flowing in response to variations in current topography. Such flows are at a very low rate resulting from the low permeability of the BVG, from the east towards the west coast.

Since the structure of the BVG is largely controlled by faults, groundwater flow in the BVG is expected to be overwhelmingly controlled by the network of fractures. The three main fractures (fault systems) are NNW - SSE, NW - SE and ENE - WSW, and are generally steep or vertical. The fracture intensity is between $10 m/m^2$ and $17 m/m^2$, the frequency of the faults is 0.66 faults per meter according to a study on the BVG core of Borehole 4 (NIREX, 1993d). There are more faults in the BVG top than towards its base. From the borehole tests (NIREX, 1993d), there is no enhanced hydraulic conductivity where the major faults intersect boreholes, and changes in head do not occur at the precise locations of the faults. The statistical treatment by NIREX (NIREX, 1993d) suggests that there is no particular bias towards structure type or orientation for explaining the flowing features, and neither are fracture envelopes to faults associated with flowzones. This implies that it is not necessarily fault zones that are associated with higher flowing rates. On the average, the BVG which contains logged faults is more hydraulically transmissive, by about $1^1/_2$ orders of magnitude, than the BVG intervals without logged faults.

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AGE	GROUP	FORMATION	LITHOLOGY	THICKNESS (m)
QUATERNARY			Tills, sands,clays and gravels	0-300
TERTIARY			Basaltic Intrusions	
JURASSIC	Lias		Grey Mudstones and limestones	500
TRIASSIC	Mercia Mudstone Group		Red Mudstones, Siltstones and Halite	<3700
	Sherwood Sandstone Group	Ormskirk Sandstone	Sandstones,mainly red, fine to medium- grained	250
		Calder Sandstone		650-1000
		St Bees Sandstone		<1000
PERMIAN		St Bees Shales	Red Mudstones Siltstones	0-200
		St Bees Evaporites	Anhydrite, Halite and Dolomitic Limestone	0-200
		Brockram	Breccia	0-220
		Collyhurst Sandstone	Sandstone	
	Variscan Deformation			
CARBONIFEROUS	Variscan Deformation			
	Coal Measures		Siltstones, Mudstones, Sandstones, Coals	<1500
	Hensingham Group and Millstone Grit		Siltstones, Mudstones, Sandstones, Limestones	50-2500
	Carboniferous Limestone		Limestones, Siltstones, Mudstones, Sandstones	200-5000
DEVONIAN	Late Caledonian (Acadian) Deformation and Intrusions			
SILURIAN	Windermere Group	Kendal Subgroup	Cleaved Sandstones Siltstones and Mudstones	<4500
		Coniston Subgroup		<2000
		Tranearth Subgroup		<1100
		Stockdale Subgroup		<150
ORDOVICIAN		Dent Subgroup		30-300
	Borrowdale and Eycott Groups		Basalts, Andesites, acites; Extrusive, pyroclastic and volcaniclatic rocks	<6000
	Skiddaw Group		Strongly cleaved sandstones, Siltstones and Mudstones	c. 5000

Table 2.1 Geological Sequence in the Sellafield Region: (after NIREX Report No 524)

Mineralising Episode	Principal associated minerals	Dominant type of mineralisation
ME1	K-feldspar/adularia, ± quartz, chlorite, albite, hematite	**Silicate**
ME2	**Quartz** ± epidote, calcite, apatite, K-feldspar, albite, sericite, hematite	**Silicate (& carbonate)**
ME3	**Pyrite** ± traces of chalcopyrite, arsenopyrite, marcasite, galena, sphalerite, Bi-Se sulphosalts and quartz	**Sulphide (& silicate?)**
ME4	**Anhydrite** ± barite, fluorite, hematite, quartz, siderite(?) K-feldspar	**Sulphate**
ME5	**Albite, K-feldspar, kaolinite, illite** ± hematite	**Silicate**
ME6	**Calcite, dolomite** ± barite, fluorite, hematite, pyrite, galena	**Carbonate** ± **sulphate**
ME7	**Illite clay and hematite**	**Silicate & oxide**
ME8	**Mn- and Fe-oxides/oxyhydroxides**	**Oxide**
ME9	**Calcite** ± pyrite, anhydrite, gypsum	**Carbonate** ± sulphate, sulphide

Table 2.2 Mineralisation chronology in the Sellafield area (after Milodowski, 1995)

Hydraulic Conductivity K (m/s^{-1})		Calder Sandstone	St Bees Sandstone	St Bees Shale	St Bees Evaporite	Brockram	Carboniferous Limestone	BVG
Field tes	K	1×10^{-7}	2×10^{-8}	2×10^{-9}	1×10^{-10}	6×10^{-10}	5×10^{-8}	1×10^{-10}
Core test	K_h	4.8×10^{-8}	2×10^{-8}	8×10^{-11}	7×10^{-11}	4×10^{-10}	3×10^{-11}	4×10^{-11}
	K_v	2.1×10^{-7}	5×10^{-8}	3×10^{-11}				
	K_h/K_v	2.3	0.5	2.7				
Porosity		0.195	0.116	0.028	0.017	0.042	0.012	0.008

Table 2.3 The hydraulic conductivity and porosity of the rocks in the Sellafield obtained from the measurements (median values) from NIREX

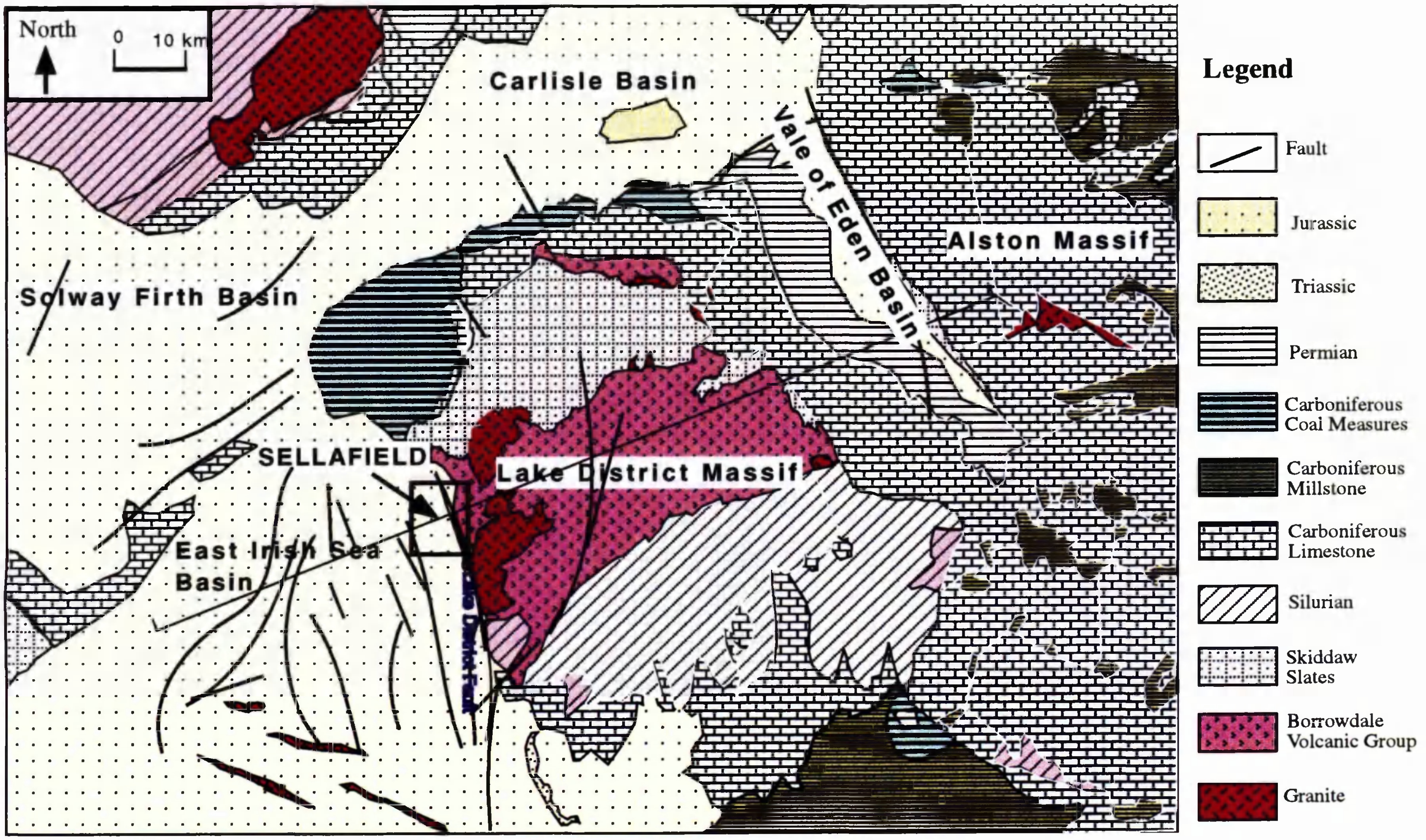

Figure 2-1 Geological setting of West Cumbria

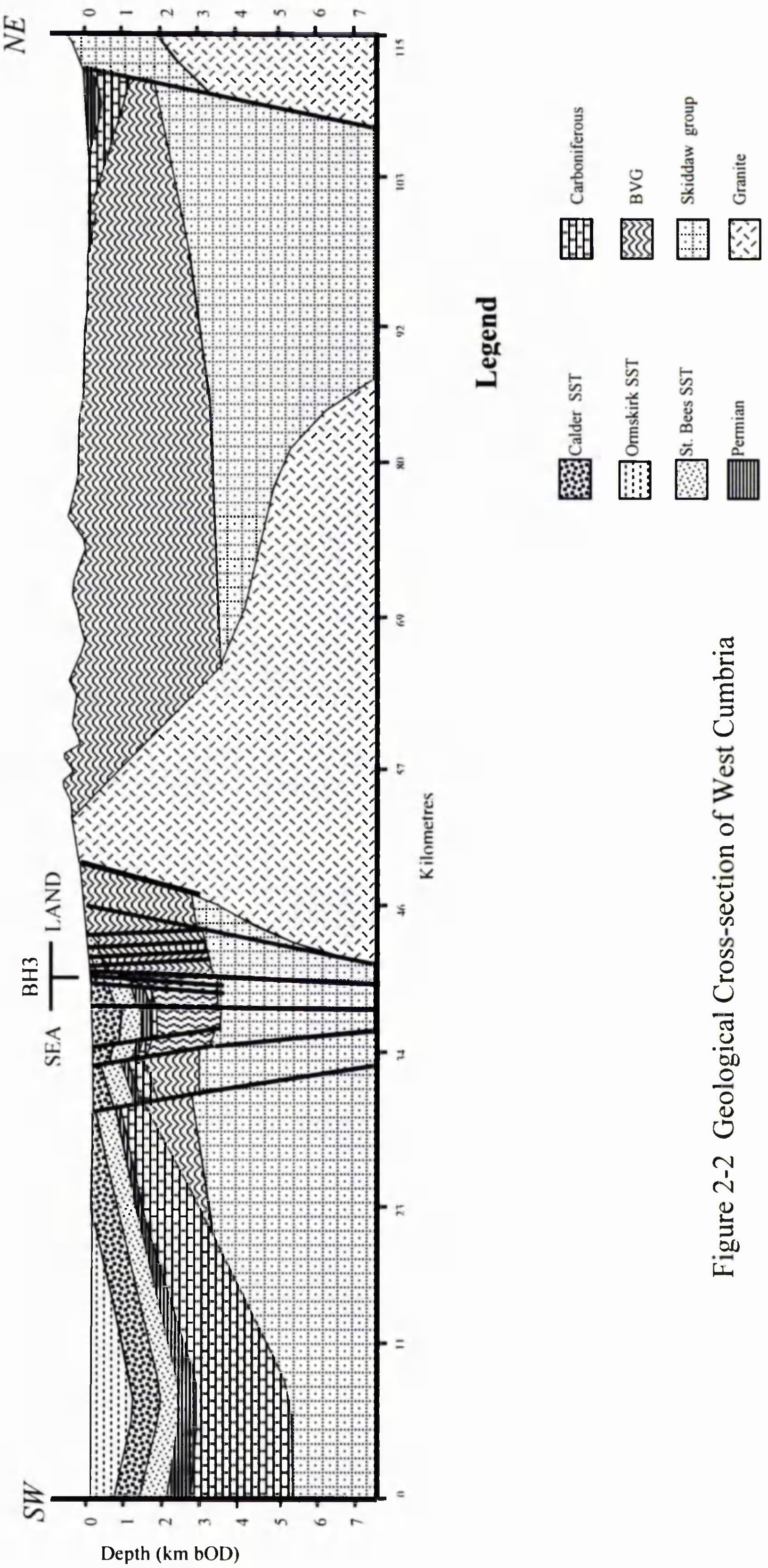

Figure 2-2 Geological Cross-section of West Cumbria

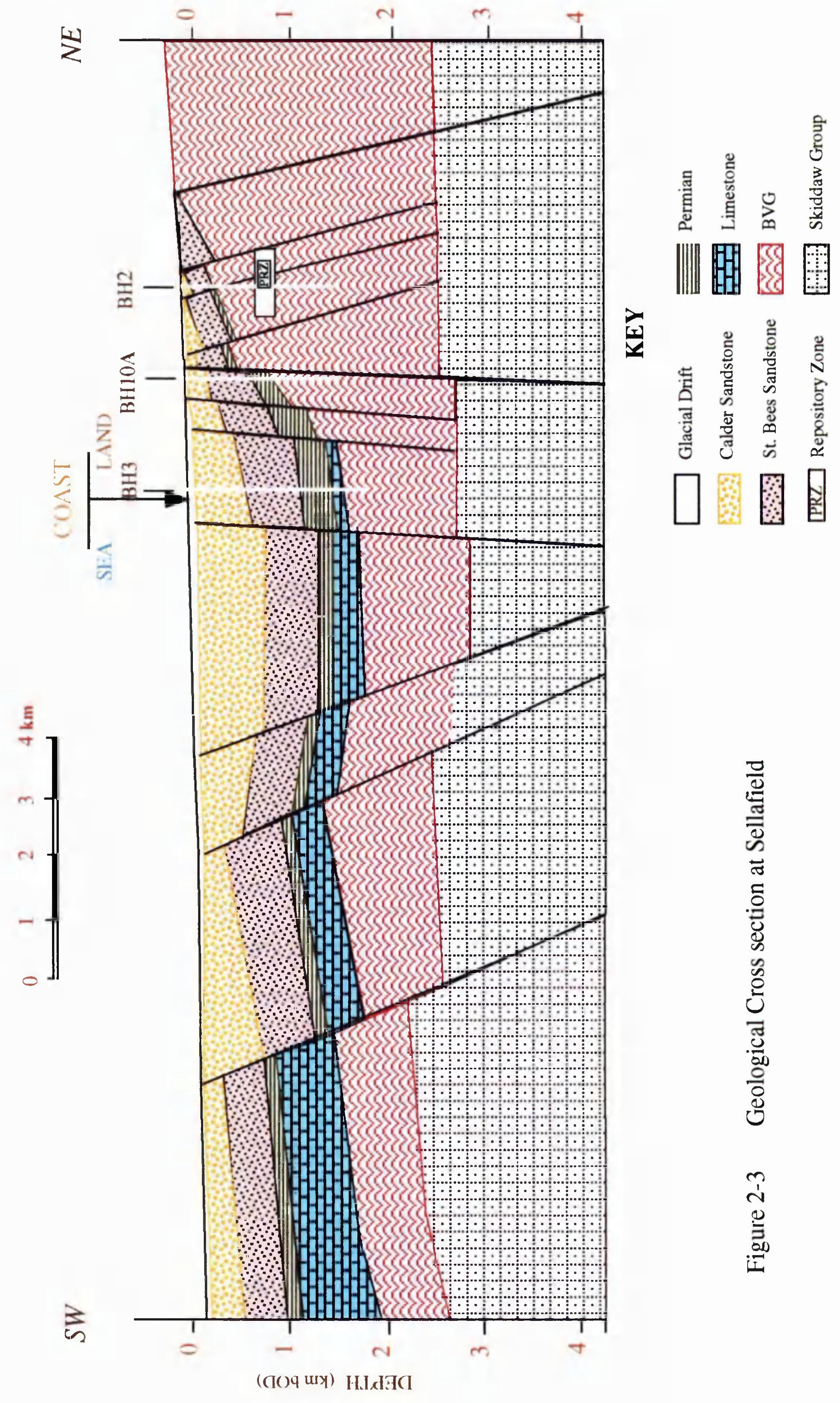

Figure 2-3 Geological Cross section at Sellafield

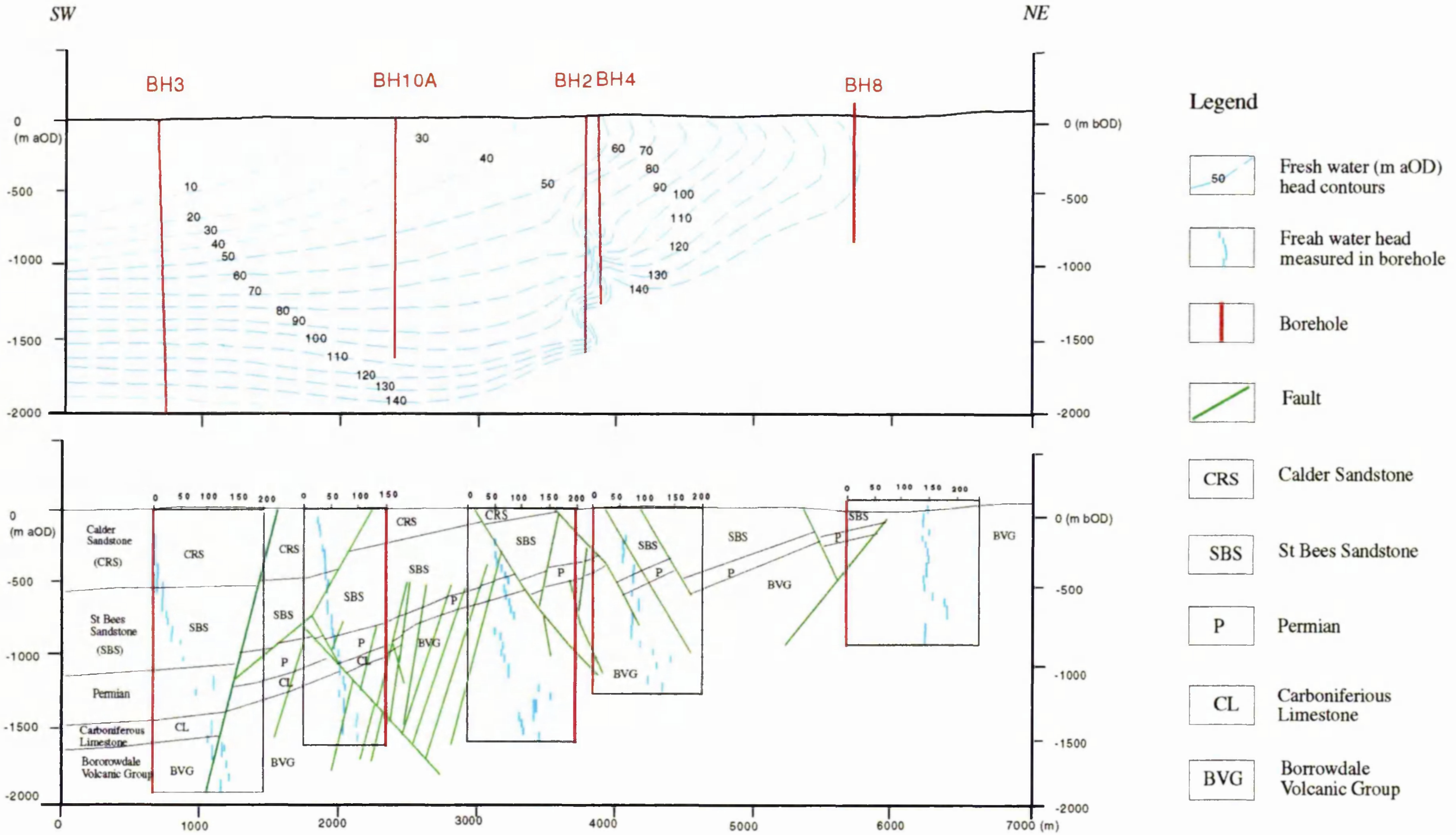

Figure 2-4 Fresh water head distribution along west-east cross section

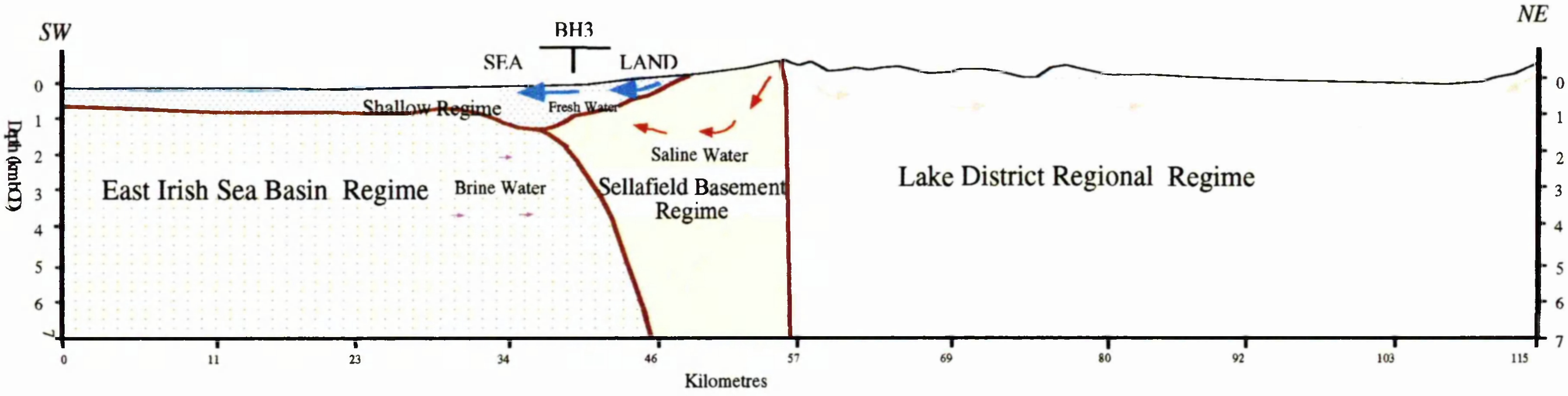

Figure 2-5
Regional Groundwater Regimes
Division in West Cumbria

Chapter 3

NUMERICAL MODEL OF GROUNDWATER FLOW

1 INTRODUCTION

Assessment of the safety of the disposal of radioactive waste in the deep subsurface relies to a large extent upon an understanding of radionuclide transport. The assessment of a particular repository site relies upon an overall performance and risk simulation. Part of the input to such overall risk is the movement of groundwater, and its potential to dissolve radionuclides from a repository and transport them towards the surface. The natural pathway for radionuclides from waste in an underground repository to the biosphere is dissolution and transport by flowing groundwater. Radionuclides released from the radioactive waste repository are transported by groundwater in a very complex network and may eventually travel to the near surface. Numerical modelling makes it possible to simulate the long term migration of radionuclides from the Potential Repository Zone (PRZ) to the biosphere. A groundwater model represents a simplified version of the real system of groundwater flow such that the model approximately reproduces the excitation-response of the real system. Creating efficient numerical models requires quantified knowledge of various environmental, geological, and hydrogeological parameters. This chapter emphasises the basic concepts of constructing a groundwater flow model. Methods of elucidating input parameters are discussed in chapter 4 and the mass transport model is presented in chapter 6.

Construction of a hydrological model can be considered in five steps, these are:
—conceptualisation
—determination of parameters
—uncertainty analyses
—calibration and prediction
The processes have been applied in hydrogeology, with various degree of success, to standard aquifers (Neuman, 1990). However, their application to regional low permeability rocks is very difficult due to lack of experience, scarcity of data, long prediction times, etc.

Conceptualisation of a model structure refers to the definition of parameter distributions within the model and boundary conditions at the edges of the model. It must encompass the physical flow processes envisaged to occur, together with identifying a geological structure to the model. In a somewhat narrower but more systematic sense, model structure identification implies expressing the model in terms of a finite number of unknowns usually called model parameters. These parameters controlling the processes may be variable in space. In some cases parameters, for example, hydraulic conductivities, may also vary in time, or depend on heads (Carrera, 1993). Usually, data are scarce so that such variability cannot be expressed accurately. Therefore, it is necessary to make some assumptions in order to simplify the variations of parameters and boundary conditions. These assumptions are reflected in the model structure and inevitably influence the accuracy of the modelling (NEA/SKI Symposium, 1990). Therefore, any model has to be calibrated and validated before it is used to make predictions.

Numerical modelling of groundwater flow started as early as the 1930's (Hayakorn and Pinder 1983). With the development of computer technology, numerical modelling has spread rapidly since the 1960's and essentially the 1970's. The first article applying the finite element method to groundwater was written in 1977 by G.F. Pinder (Pinder, 1977). At the Sellafield site, numerical modelling of the groundwater flow system is still at an early stage. There has been a series of models developed at Sellafield (Heathcote *et al,* 1996). However all of them have been small scale and shallow depth, mainly to examine fresh water. None of these models can represent the actual deep groundwater flow system beneath the area where the potential repository site was to be located. Furthermore, none of them has been either calibrated or validated. The modelling study presented in this thesis is believed to be the deepest and longest regional simulation. Consequently, this permits investigation of regional flow processes, rather than being restricted to local investigations.

There are many unanswered questions in understanding groundwater flow systems at Sellafield. These include reproducing the groundwater head in the repository site, the hydraulic properties of faults, the origins of saline water, and the groundwater age. A vertical cross section model constructed by NIREX tried to model the saline water in the potential repository zone, but the modelled water head could not match the measured values in the deepest Borehole 2, and it failed to reproduce the groundwater head in the repository site (NIREX, 1993). More satisfactory models are likely to be required to permit development of groundwater flow models that can satisfactorily reproduce observed patterns of head and salinity. Hence it is still necessary to make a further study in modelling groundwater flow in this region and to help understand the assessment of potential risk of nuclear waste dissolution in groundwater and its migration towards the surface.

The models presented in this thesis progress through various stages towards a more complete understanding of the groundwater flow system at Sellafield. To understand the regional groundwater flow in West Cumbria, a two-dimensional numerical model based on OILGEN (Garven, 1989) was used. This finite-element model permits coupling of rock properties, water properties, and flow resulting from potential differences, including consideration of heat transport. This study focuses on reproducing the regional groundwater flow and local flow at a repository site, in particular, the water head and flow pattern in the BVG that is intended for the repository volume. Specific investigations include the sensitivity of rocks and fault permeability, and salinity or density in controlling fluid flow in West Cumbria, and how these may influence the flow path of groundwater transporting radionuclides. A regional section 115 km long and 7.5 km deep has been constructed. Determination of the model parameters is a critical point, especially in such a regional model, where the borehole data are scarce. This determination has been carried out through sensitivity tests that will be discussed in chapter 4. In order to choose a realistic suite of parameters which enable an understanding of geological factors which influence the fluid flow in West Cumbria, the modelled freshwater head profiles must be calibrated by comparison with measured values from wells. This tests the credibility of the input values and geometries. In developing these models, the concept of the model and the geometry of the model have to be progressively modified from time to time according to test results. This chapter emphasises the conceptualisation and numerical creation of the model.

2 CONCEPTUAL MODEL

2.1 Aim of conceptual model

The first step in the procedure of modelling is the construction of a conceptual model of the problem and the relevant hydrogeological domain. The aim of the conceptual model is to encapsulate the understanding of the hydrogeological system. This consists of a set of assumptions which reduce the real problem and real domain to a simplified version that is acceptable in view of the objectives of the modelling.

A conceptual model is a hypothesis for how a system or process operates, which is then quantified by a numerical model. The conceptual model helps to define a numerical model and interpret the data from hydrogeological investigation

(Kazda, 1990). It is the most important and difficult step in modelling. Even a minor misjudgment or wrong presumption will cause totally wrong calculation results. In spite of the large amount of data available, a conceptual model is essentially qualitative in nature. Thus, more than one conceptual model may be available to describe the system (Black & Brightman, 1996). Numerical modelling is then used to develop a general understanding of the hydrogeological system, by improving the conceptual model and determining the parameters of the rocks. The whole process is iterative, leading towards improved modelling.

The difficulties of conceptualisation are generally increased in low permeability rock formations that may be the targets for radioactive waste repositories. This is because less hard data are expected to be available, and because small scale tests may not represent the large scale rock. Tests might be less informative than in larger permeability environments. There are also difficulties in choosing deterministic equivalents to flow paths, or stochastic assumptions of matrix permeability rather than fracture flows. The experience of hydrogeologists in this field is very limited (Carrera *et al*, 1993). The process and properties used to define the hydrogeological regime in the conceptual model relate to the following items:

—the geometry of the boundary of the investigated domain
—the hydrogeological properties of rocks
—the mode of flow in the regime (two dimensional, porous medium)
—the properties of water (with reference to its density and viscosity)
—the effect of temperature on density and viscosity
—the forces driving groundwater flow

2.2 Groundwater flow medium

A key assumption is that groundwater flow through rocks can be treated as flow through a porous medium when rocks are evaluated at a regional scale (Furbish, 1997). It is assumed that such porous media are homogenous and anisotropic. This approach has been tested by other groups (Tompson, 1993; Moreno and Neretnicks, 1993). The justification for this approach is that fractures flowing groundwater have been observed in cores from the Sellafield site, the spacing of small fractures is often less than 2 m (NIREX, 1993). This spacing is always less than 20 m and less than the finite element grid blocks in our modelling. In this case, the rocks in Sellafield should be treated as a porous medium and they consist of:

1) Basement of Lower Palaeozoic age (c. 510-395 million years), exposed in the Cumbria-Mountains (Lake District Block). It comprises: Eskdale Granite Intrusion, Borrowdale Volcanic Group (BVG) and Skiddaw Slate

2) A cover sequence of sedimentary rocks of Carboniferous (c. 350 Ma) to Triassic (>210 Ma) age, in the coastal belt and offshore (East Irish Sea basin). These include:

Triassic Sherwood Sandstone Group
—Ormskirk Sandstone
—Calder Sandstone
—St. Bees Sandstone
Permian
—St. Bees Shale,
—St. Bees Evaporite,
—Brockram Breccia
Carboniferous Limestone

3. Fault zones, including faults in 'Sedimentary Rocks' and faults in 'Basement'.

4. A variable thickness of poorly consolidated glacial and post-glacial sediments, overlying the older rocks.

2.3 Groundwater flow regimes

The groundwater flow system can be divided into three basic regimes based on the hydrogeological borehole investigations (Bath *et al*, 1996). This division coincides with the distribution of salinity in the groundwater (See Figure 3-1).

—East Irish Sea Basin Regime. These are brine waters (TDS>100 g/l) and the flow is almost static. This regime occurs in the cross section from Borehole 3. The western boundary of the regime is not seen. The source of the brines is from dissolution of evaporites within the Irish Sea Basin. Brine observed in the deep boreholes at Sellafield is assumed to continue to considerable depth. The uppermost and eastern boundaries are intersected by the Coastal Plain and Basement-Hills regime respectively.

—Coastal Plain Regime. This is a fresh water (TDS < 1 g/l) system locally distributed east of the coast and within the near surface rocks. The westwards flow rate is moderately high and is driven by topography. This regime is recharged from precipitation onto hills in the east, and discharged into the sea near the coast. The lower boundary of the fresh water regime coincides with the Brockram Rocks. The boundary between the Coastal Plain regime and the Hills-

Basement regime is taken as the base of the St. Bees Sandstone. The top of the boundary is the groundwater table, generally in the superficial glacial Drift.

—Hills-Basement Regime (Lake District Regime). The groundwater is expected to be brackish or saline (TDS 10-100 g/l), and largely topographically driven; this regime contains the Potential Repository Zone (NIREX, 1993). Flow is mainly recharged from hill area precipitation and discharged to the other regimes. Regionally, the rainfall precipitation recharges the BVG and granite; thereafter the groundwater is expected to flow westwards and downwards. Groundwater flow is expected to be very slow in the regime due to the low hydraulic conductivity of the Basement. As a result, water-rock interaction may take place, which might increase the amount of total dissolved solids. The Lake District hills produce a groundwater divide, which represents the eastern boundary of the Hills-Basement Regime. The western boundary is defined by the brines from the East Irish Sea Basin Regime. The west-upper boundary is overlain by the Coastal Plain Regime.

2.4 Regional Cross Section

There is a general geological and topographic East-West symmetry about a cross section perpendicular to the coastline at Sellafield, so there is symmetry about groundwater flow. Consequently, it is convenient to use a two dimensional cross section model to study the groundwater flow in this area, presuming that the groundwater flows at right angles to the line of the coast. A cross section is constructed from the East Irish Sea Basin to the Lake District Block and Carlisle Basin, North-West perpendicularly to the coast, which is 115 km long and 7.3 km deep. This geological cross section was based on the NIREX geological data published in 1995 (NIREX, 1995).

2.5 Salinity distribution

The salinity distribution used in the models was derived from borehole data presented by NIREX report (NIREX, 1993). In the East Irish Sea Regime, the salinity distribution was based on solute concentrations measured in Borehole 3. All nodes within the finite element mesh down to 400 m bOD were assigned seawater concentration. From 400 m bOD to 1000 m bOD, the salinity increased linearly to a value equal to that measured in Borehole 3. Below this depth, all nodes kept the same gradient until a maximum value of 1200 kg/m^3 was reached. East from Borehole 2, the salinity concentration was based on Borehole 2 data. The mesh nodes from surface down to 300 m bOD were assigned to be freshwater, below this the concentration increased linearly with a constant gradient to a value at depth of 1000 m bOD, where a value equal to that measured in Borehole 2 was reached. Between Borehole 3 and Borehole 2, the concentration values were interpolated to rely on density measurements from Borehole 3, Borehole 10A and Borehole 2.

The boundary between individual salinity systems may be influenced by the changes of geological conditions. It was suggested that the boundary between the Irish Sea Basin Regime and the Coastal Plain Regime be generally in equilibrium with current conditions. Although it is difficult to judge whether the boundary between the Irish Sea Basin Regime and the Hills-Basement Regime is in equilibrium or not, it is likely that it might be relatively static because of the extremely low permeability of units in this area and inferred static flow condition. Due to a lack of potential flow drive from the Irish Sea, the boundary movement is likely to be so slow that it is negligible in this regional modelling.

3 Numerical Model

Hydrogeological modelling is a method designed to simulate some aspects of a real hydrogeological system. For practical reasons, the modelling process has to select those features which most significantly affect the phenomenon under study. In general, the most important processes affecting the water movement are well known, and four types of information are usually considered in a hydrogeological model.

(1) Groundwater properties
(2) Groundwater flow patterns and velocity
(3) Temperature
(4) Mass concentration

3.1 Fundamental concepts

Basically in hydrogeological studies, two conservation laws are generally considered (Domenico *et al*, 1983):

1. Law of conservation of mass (continuity principle)
2. The law of conservation of energy (first law of thermodynamics)

A third basic concept is the second law of thermodynamics, this of equal importance when one is interested in the nature of loss in mechanical thermodynamics, or when one is investigating the establishment of chemical equilibrium between mineral matter and aqueous solutions.

As early as the first half of the nineteenth century, it was recognised that the velocity of laminar flow of water in porous media is proportional to the slope of the hydraulic gradient (Domenico *et al*, 1990). Darcy's statement of the law is

$$Q=KA\frac{h_1-h_2}{L} \tag{3-1}$$

where K is hydraulic conductivity (length time^{-1}) and contains properties of both the medium and the fluid, A is the cross section area (length^2), L is the filter length (length), (h_1-h_2) is the difference in water level elevations (length) in the inflow and outflow.

In a non-compressible homogeneous and anisotropic porous medium, for vertical plane flow where x, y denote horizontal and vertical direction respectively, hydraulic conductivity is defined by

$$\mathbf{K}=\begin{bmatrix} K_x & K_{xy} \\ K_{xy} & K_y \end{bmatrix}$$

Darcy's law has the form

$$\mathbf{V}=-\mathbf{K}\nabla h$$

where $\mathbf{V}$ is the seepage velocity (length time^{-1}), $\nabla$is the Hamilton operator, h is the total head (length) defined as

$$h=y+\frac{p}{\rho g}$$

where y is the elevation of the point (length), g is the gravitational acceleration (length^{-1} time^{-2}), p is the fluid pressure (mass length^{-1} time^{-2}), ρ density of water (mass length^{-3}).

3.2 Fundamental equations of groundwater flow

3.2.1 *General motion equation*

Generally, in a non-deformable porous medium, the equation most often cited as Darcy's law is written

$$\mathbf{q} = -\frac{\mathbf{k}}{\mu}(\nabla \mathrm{p} + m \mathrm{g} \nabla \mathrm{y}) \tag{3-2}$$

where **q** is the volumetric flow rate of fluid (length^3 time^{-1}), **k** is the intrinsic permeability tensor (length^2) and contains properties of the medium only, μ is the dynamic viscosity of the fluid (length^{-1} time^{-1}), m is mass per unit volume of fluid (mass length^{-3}).

3.2.2 *Streamline and stream function*

In practice, there is an alternative description of groundwater flow based on a stream function. In two dimensional flow, the ideal flow is irrotational flow and the governing equation of the streamline takes the form

$$d\Psi = q_y dx - q_x dy \tag{3-3}$$

where Ψ is the stream function, and q is the volumetric flow rate of fluid per unit volume rock withdrawn. The instantaneous curves at every point, which are tangential to the velocity vector at that point, are called streamlines. In steady flow, pathline and streamline are identical since velocities do not change with time.

3.2.3 *Basic mass balance equation*

Using the mass conservation law, we can obtain the basic continuity (or mass balance) equation in a steady flow, when both water and solid matrix are assumed to be incompressible:

$$\nabla \cdot \mathbf{q} = 0 \tag{3-4}$$

By introducing Darcy's law (3-2) into (3-4) we can get:

$$\nabla \cdot \frac{\mathbf{k}}{\mu}(\nabla p + \rho g \nabla y) = 0 \tag{3-5}$$

In Cartesian coordinates, assuming that the material is anisotropic and homogeneous, the continuity equation becomes:

$$\frac{\partial}{\partial x}(K_x\frac{\partial h}{\partial x})+\frac{\partial}{\partial y}(K_y\frac{\partial h}{\partial y})=0 \tag{3-6}$$

and the partial differential equation that describes the flow in terms of Ψ is

$$K_x\frac{\partial^2\Psi}{\partial x^2}+K_y\frac{\partial^2\Psi}{\partial y^2}=0 \tag{3-7}$$

3.2.4 *State Equation*

The third equation is the isothermal equation of state of the fluid:

$$\rho=\rho_0\, e^{\beta(p-p_0)} \tag{3-8}$$

$$\mu=\mu_0\, e^{\beta(p-p_0)} \tag{3-9}$$

Where β is the coefficient of fluid compressibility (mass^{-1} length time^{-2}), p is the pressure (mass length^{-1} time^{-2}).

3.3 Heat Transport in Groundwater Flow

There are three processes of heat transport in a porous medium: conduction, convection, and radiation. Similar to Darcy's law in fluid flow, there is a Fourier's law to describe heat conduction as

$$H=-\kappa_e\nabla T \tag{3-10}$$

where H is the heat flux, T is temperature, κ_e is an effective thermal conductivity. In the two phase case, fluids and solids, the accepted relationship is (Furbish, D. J., 1997):

$$\kappa_e=n\kappa_f+(1-n)\kappa_s \tag{3-11}$$

where f and s refer to the fluids and the solids, respectively, and n is the porosity of the rocks. Thermal dispersion is normally incorporated in the transport parameter κ_e because it has the same effect as an increase in the effective thermal conductivity.

Based on the first law of thermodynamics, we can obtain equations of energy conservation for the conductive-convection, which is as

$$-\kappa_e \nabla^2 T - \rho_w c_w q \cdot \nabla T = 0 \tag{3-12}$$

where **q** is the volumetric flow rate of fluid, ρ_w and c_w are the density and specific heat of the liquid. In equation (3-12), the velocity field and the heat field are coupled and could only be solved iteratively. The solution of these equations needs certain boundary and initial conditions.

3.4 Boundary Conditions

The vertical side boundaries and the bottom boundary of this model are taken to be no-flow boundaries. The top boundary follows the ground surface or stays at sea level west of the coast. Flow is permitted across this boundary. The western boundary is 39 km away from the coast, consequently it should have a minimal boundary effect on the groundwater flow in the PRZ. The eastern boundary is similarly chosen to be 70 km distant from the PRZ so that all the possible groundwater recharge to the PRZ can be involved in this model. Salinity distributions are based on solute concentrations measured in Borehole 3, Borehole10A, and Borehole 2, as discussed previously.

4 FUNCTIONAL DISCRETISATION

To solve the equations in the modelling of groundwater flow, the Galerkin finite-element method is used to solve the partial differential equations (Kazda, 1990). The finite element method is a numerical method whose rise and development has been enabled by the rapid development of computers. In this method any set of continuous functions can be approximated by a discrete model which consists of a set of values of the given functions (eventually with its derivatives) at a finite number of preselected points in the selected domain, together with piecewise approximations of the function over a finite number of connected distinct subdomains.

Using the simplest element with the Langragian interpolation, the domain (Ω) to be calculated is divided into a set of triangular finite elements with N nodal points. In every element A_r, the function is approximated by means of local interpolating functions. In this study, a linear interpolating polynomial basis function φ_r is introduced for each point, which has an interpolating polynomial form and the following relation (Kazda, 1990):

i) $\varphi_r = a_r + bx + cy \qquad r \in \Omega$
ii) $\varphi_r(A_r) = 1;\ \varphi_s(A_s) = 0;\ \varphi_t(A_t) = 0 \qquad x, y \in A_r$
iii) $\varphi_r = 0; \qquad x, y \notin A_r$

Using the interpolating functions, the groundwater head h (x, y) approximation to all the elements can be expressed over the domain as:

$$\mathrm{h(x,y)} = \sum_{r=1}^{N} \mathrm{h_r \varphi_r (x,y)} \tag{3-13}$$

Approximation (3-13) can be substituted into equation (3-6) or (3-12) and both sides multiplied with $\varphi_i = (x, y)$, then integrated all over the domain Ω. Using Green's theorem and inserting boundary conditions, we can obtain a system of algebraic equations

$$\mathbf{A}h + \mathbf{B} = \mathbf{Q} \tag{3-14}$$

where h is the groundwater head to be solved, $\mathbf{A}$ is the conductive matrix $(n_p \times n_p)$ that is symmetric, $\mathbf{B}$ is the buoyancy vector, and $\mathbf{Q}$ is the flux vector.

Similarly using this scheme for the heat equation (Garven and Freeze, 1984), we get another system of algebraic equations for temperature.

$$\mathbf{S}T = \mathbf{F} \tag{3-15}$$

where T is the temperature to be calculated, $\mathbf{S}$ is the conductive matrix $(n_p \times n_p)$ that is asymmetric and $\mathbf{F}$ is the flux vector.

The solution of the system of equations (3-13), (3-14) and (3-14) can be easily obtained by means of Gaussian elimination.

5 SOLUTION PROCEDURE

I have constructed a regional 2-D cross section model to represent the regional groundwater flow and heat transport. This cross section starts from the East Irish Sea, goes north-eastward through Sellafield, and through the Lake District Block, ending at the Alston Block. The section is 115 km long and 7.3 km deep. To numerically discretise the region, 3750 nodal points and 7500 triangular elements are used. The finite-element mesh is shown in Figure 3-2.

The numerical procedures are outlined in Figure 3-3. Firstly, all the data are input and the data arrays are filled; secondly, the steady-state groundwater head is computed assuming no salinity and temperature gradient. Thirdly the Darcy velocity in each element is calculated. Then the steady-state heat equation is solved. With the newly calculated values of pressure, temperature and the specified salinity profile, the fluid densities and viscosities are computed from the equation of state, then the groundwater head is recalculated. After that all the steps are repeated until the temperature difference between subsequent iterations falls below 1% from all nodes.

6 SUMMARY

The construction of numerical models is a progressive process. A conceptual model is not trivial, both to define a numerical model, and interpret the data from a hydrogeological investigation. It is the most important and difficult step in modelling. Even a minor misjudgment or wrong presumption will cause a totally wrong calculation result. The difference between my regional model and other workers local model is that the boundary of my regional model is wider and much more recharge is considered. The area of interest (the repository zone) is a long way from edge effects at model boundaries. In particular, the low permeability basement and hills area were involved in the regional models, which are very important to the deep flow systems. There are two sources of salinity, one is from the East Irish Sea Basin Regime. These are brine waters and the flow is almost static driven by basinal process. The other source is from the Hills-Basement Regime, where groundwater flow is very slow in the regime due to the low hydraulic conductivity of the Basement. As a result, water-rock interaction may take place, which might increase the amount of total dissolved solids.

The application of numerical models to regional low permeability rocks is very difficult due to lack of experience, expected scarcity of data, and long prediction horizons. There are many unanswered questions in groundwater modelling at Sellafield. More satisfactory models are likely to be required to permit the development of groundwater flow models that can satisfactorily reproduce observed patterns of head and salinity. This study was divided into several stages, trying to investigate these biases in the modelling and reproduce both local and regional groundwater flow systems. In particular, the water head and flow pattern in the BVG where the repository volume stands. To deal with deep underground water flow modelling, the finite-element method was used to discretise the equations. This study also tackled features of water properties, flow patterns associated with streamline, heat transportation as well. In order to minimise the effect of boundary conditions on the calculation, the side boundaries were chosen over 50 km from the repository area.

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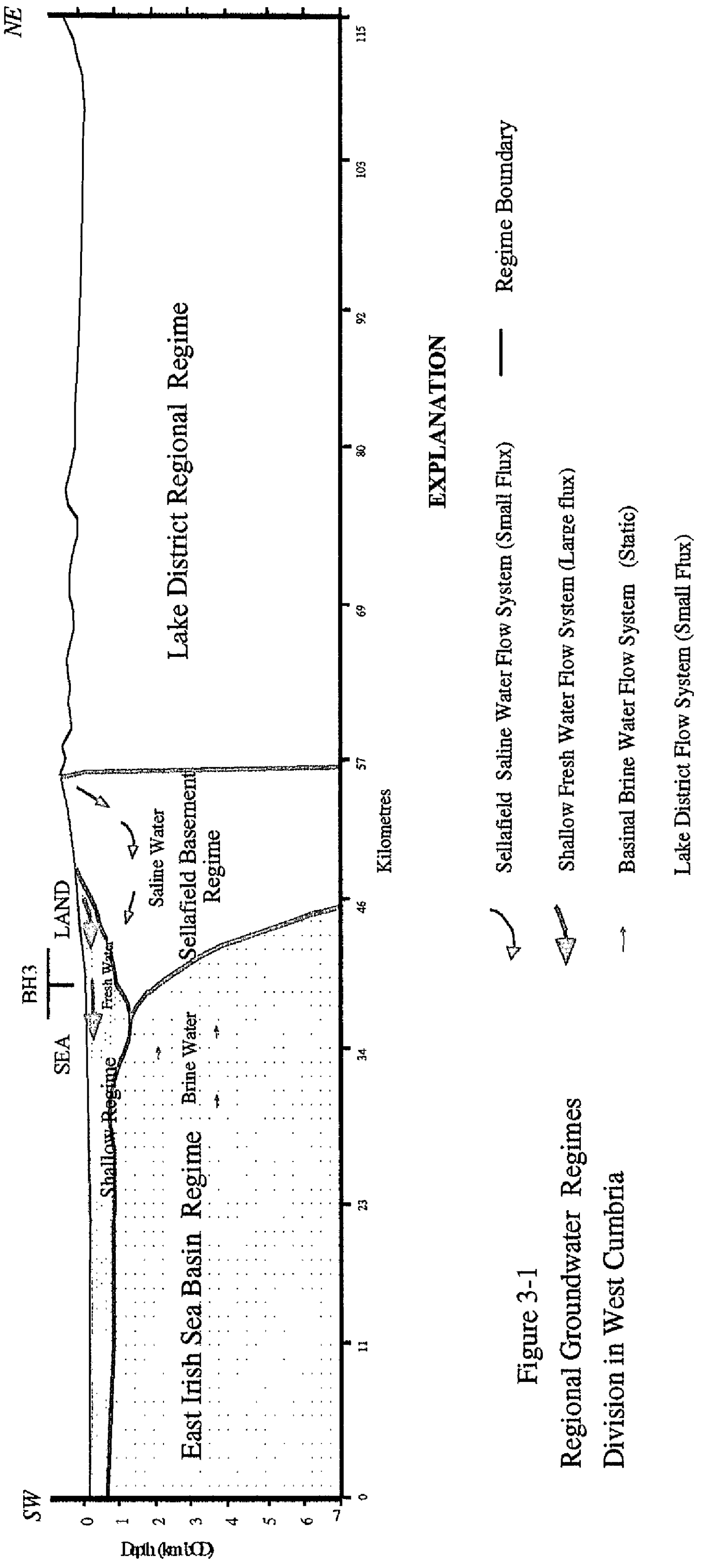

Figure 3-1
Regional Groundwater Regimes
Division in West Cumbria

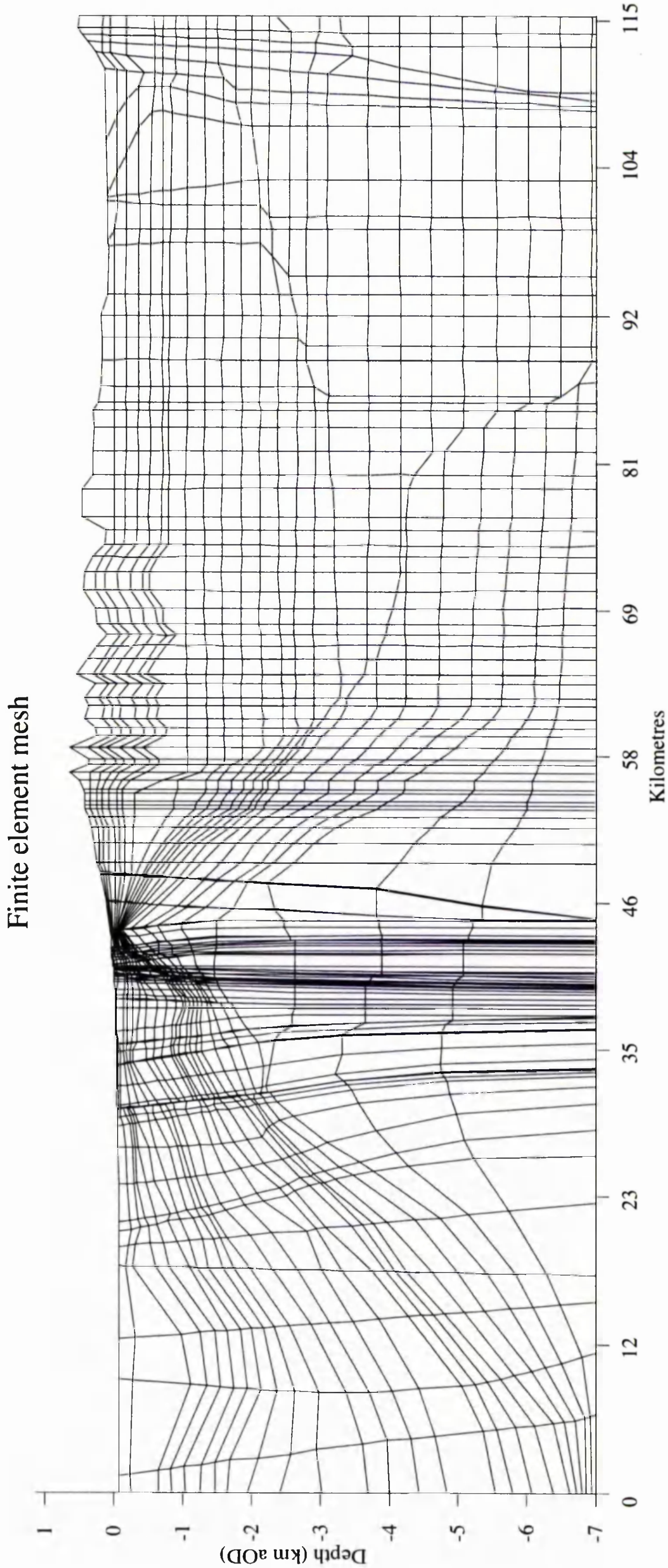

Figure 3-2 The finite element mesh used in the West Cumbria ground water model

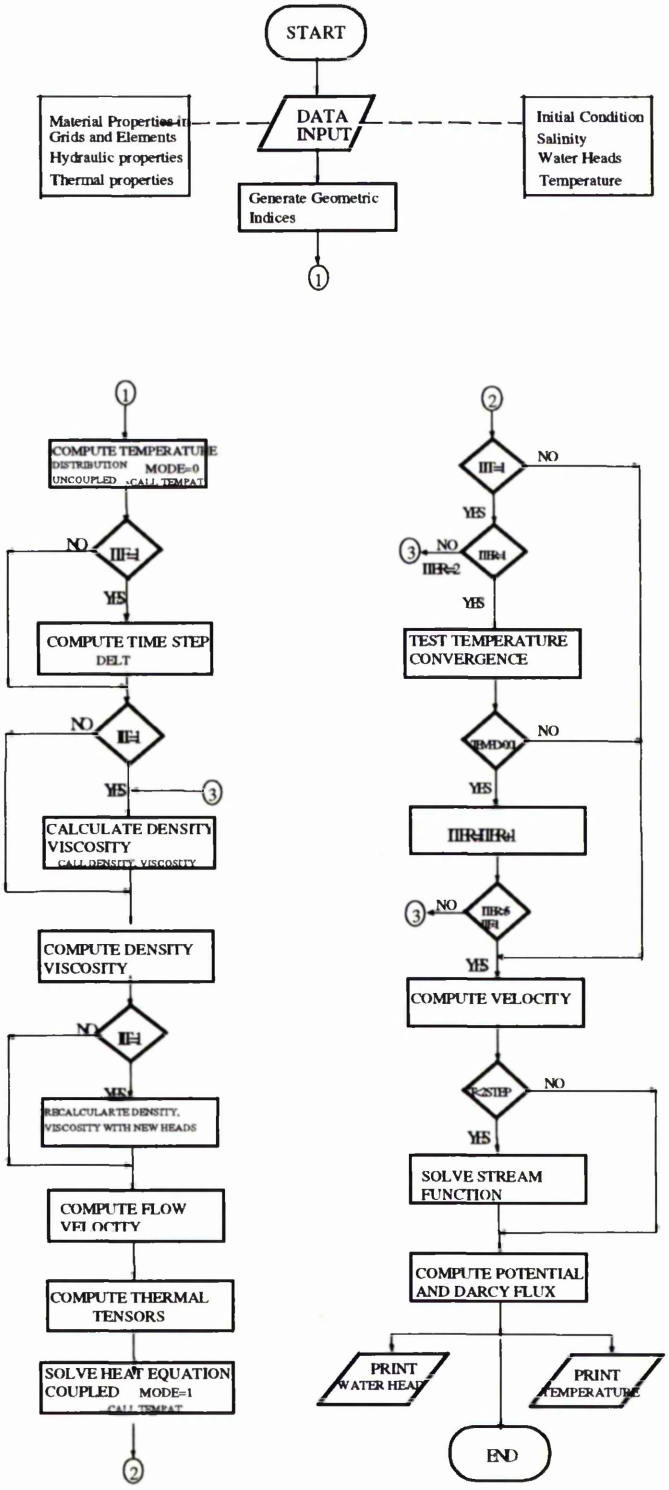

Figure 3-3 The flow chart of the groundwater flow model

Chapter 4

DETERMINATION OF PETROPHYSICAL PROPERTIES

1 INTRODUCTION

Creating efficient numerical models requires knowledge of various environmental, geological, and hydrogeological parameters. These all exhibit large uncertainties due to the limited number of exploration and investigation boreholes, and the natural heterogeneity of underlying geological formations at the waste site. Analysis of parameters fed into the groundwater model plays an important role in the assessment of the safety and the performance for a proposed repository. Any groundwater model that is to be used for modelling safety predictions should be calibrated (NEA/SKI, 1990). This means that the model accurately reproduces the characteristics of the natural system. As heterogeneity exists in the subsurface, restrictive or unjustified assumptions can often be made about the physical system. A complexity or uncertainty in geophysical properties can be produced by heterogeneity in formation materials and their associated properties, or constraints on the type and quantity of measurements available to characterise real systems (Carrera, 1993). Hence it is clearly desirable that the model should be checked, and the numerical model should be calibrated, so that it is shown to accurately represent the intended mathematical models and physical phenomena. One approach is to determine these uncertainties using sensitivity tests of the parameters fed into the model. In the present example, these characteristics consist of the heads measured in observation wells, and to a lesser extent, the residence ages inferred for the groundwater. In this chapter, I describe the steps that permitted me to create a calibrated model of the groundwater system at Sellafield. In particular, I consider the number and distribution of hydrogeological units, and their petrophysical characteristics (permeability and perm-anisotropy). The result is a calibrated comprehensive model.

Much of the geological information used in this study was derived from NIREX reports. NIREX has been drilling more than twenty deep boreholes since 1989 (NIREX, 1993a). Hydrogeological testing and groundwater sampling have provided additional information on the hydrogeological conditions at the site. Much of the geological and hydrogeological work undertaken by NIREX was at the leading edge of international practice, and the basic data set should be highly reliable (Knill, 1994). The hydraulic conductivity of the rocks at Sellafield has a wide range, from 10^{-3} m/yr to 1000 m/yr. Even within the same type of materials the hydraulic conductivity ranges over 5 orders of magnitude. So the determination of the model parameters is a critical point in the modelling, especially in such a regional model, where the borehole data are scarce.

NIREX have tried to avoid addressing this variability, by conducting stochastic simulations (NIREX, 1993b). But I have chosen a different approach. I seek to determine the least number of distinct hydrogeological materials, and their petrophysical properties, which allow me to create a calibrated model. My approach produces a result that is completely transparent, it is hence subject to assessment by our interested audience.

The general approach here is to perform a series of sensitivity tests to determine appropriate values for the petrophysical properties. During these tests, the data measured in deep boreholes were used to ensure that the tests were linked to the actual natural conditions. All of these tests rely on comparing the match between predictions arising from the test models, and measured values from *in-situ* boreholes. In this case modelled freshwater head profiles are compared with the values measured from wells to test the credibility of the model input values and geometry. In order to progressively increase understanding of the flow and transport processes in the area, and to make the modelling as simple as possible, the work proceeds from a simple stage to more complex ones. Emphasis is put on demonstrating the role of regional groundwater flow, in directing flow across less permeable basement to focus flow towards the PRZ and coastal discharge areas, and on examining temperature and salinity effects.

Calibration of a performance assessment model for waste repositories is expected to be particularly difficult because of the scarcity and low information content of hydrogeological data, caused by the low permeability of candidate geological formations and by the limitations that are likely to be imposed on drilling and testing. In my study these issues were resolved using a sequential process: the initial model was calibrated and the geometry of zones and the extent of material were then changed so as to reduce the difference between measured and computed heads. The parameters obtained during the sensitivity test are not certain, in fact, they can be highly uncertain. The quality of the estimation can additionally be assisted by calibration of the model using hydrogeological data and hydrogeochemical data. This will be discussed in chapter 6.

2 Hydrogeological Data

2.1 Petrophysical properties

The hydrogeological properties reported by NIREX come from the testing carried out in deep boreholes, and from analyses of cores produced during drilling. The hydraulic conductivity of the rocks was initially determined in the boreholes using 50-metre long contiguous section tests. Unfortunately, there is a considerable degree of natural variability recorded in these determinations.

There are two main sources of NIREX data on petrophysical properties: the borehole testing program, and the core characterisation program (NIREX, 1993b). The Environmental Pressure Measurement (EPM) tests in boreholes were designed to obtain the undisturbed fluid pressure in-situ. Pressure drawdowns were induced in pumping tests, and the pressure recovery curves were analysed to obtain transmissivity. These tests provide almost continuous coverage of the 50m intervals in the boreholes across all lithologies. The data set provides the largest number of statistical samples for each of the hydrogeological units.

Permeability (k) is defined as the ability of the solid matrix to transmit fluid. This depends solely on the solid matrix, and is often written as milliDarcies (mD). One milliDarcy is equivalent to 9.613×10^{-9} m/s (=0.3 m/yr) of freshwater at standard conditions.

In order to measure the permeability or hydraulic conductivity of rocks, standard laboratory methods were used to measure the porosity and gas permeability of the core samples. Statistical tests of the differences between the borehole conductivity measurements and core sample tests were undertaken. These verified the need to consider each hydrogeological unit separately, with different hydraulic conductivities for each. The core sample tests also showed detectable anisotropy in hydraulic conductivity. The hydraulic conductivities of the core tests and field hydraulic conductivities are presented in Figure 4-1.

The hydraulic conductivity also has a pronounced scale effect, which is particularly significant in the Carboniferous Limestone (Figure 4-1). The field test values are almost one or two orders of magnitude higher than those from the core tests. Accordingly, the parameters used in my models were always based on the results of the field tests.

2.2 Groundwater heads

Groundwater head is a measure of liquid potential energy expressed as the height (relative to some reference: called Ordnance Datum or sea level) of the top of a vertical column of water that would be supported by the in-situ pressure. The hydraulic head for the point comprises its elevation and the pressure head due to the overlying column of water (see equation 3-2-2). The groundwater pressures in the NIREX boreholes were determined by:
(i) Environmental Pressure Measurement (EPM) tests, these provide a semi-continuous sequence of the pressure (at a rather coarse scale);
(ii) Discrete Extraction Tests (DET), were measured immediately after drilling over variable length test sections at a specific location;
(iii) Post Drilling DET (PDDET), provided a longer-term analysis of pressure of post completion testing measured over selected intervals of the boreholes.

In general the majority of the pressures derived from the EPMs are considered reliable and reproducible by other forms of testing and measurement, and therefore could be used as the most complete data set of pressures.

Groundwater at depth in Sellafield is saline, the fresh water head expressed in situ as meters of fresh water is relative to the Ordnance Datum (OD), which is obtained by subtracting the pressure due to the column of water of variable density from the measured environmental pressure. Figure 2-4 shows the groundwater head measured in those boreholes which are used in calibration of the models.

2.3 Characteristics of the hydrogeological units

Based on the NIREX hydrogeological investigation (NIREX, 1993b), each of the lithostratigraphic units has distinctive hydrogeological properties (Table 4.1). However, some of the individual units are very thin, consequently their hydrogeological properties have been merged to be treated as a single unit. Here, I treat the St. Bees Shale, St. Bees Evaporite and Brockram, as the same unit: the Permian. Although the Carboniferous Limestone may be thin (within the borehole less than 50 m), the median value of field hydraulic conductivity for the Limestone at 5×10^{-8} ms^{-1} is more than one order of magnitude greater than that of the other units and it should be treated as a distinct hydrogeological unit. Accordingly, the minimum number of hydrogeological units at Sellafield can be divided into: Drift; Ormskirk Sandstone; Calder Sandstone; St. Bees Sandstone; Permian; Carboniferous; BVG; Fault zones.

The BVG and all other sediments were considered to be anisotropic, with the maximum conductivity being parallel to their dip in the regional east-west cross section. These units can be either combined or divided according to the model concept.

3 METHODOLOGY

From a hydrogeological point of view, the most important factors controlling groundwater flow are: (1) topography, or the water table configuration, (2) hydrostratigraphy and the resulting variations in the hydraulic properties. In this study, the emphasis was placed on determining the hydraulic properties that ultimately reproduced the observed heads. I also examined the temperature and salinity effects on the groundwater flow. The general approach here is to perform a series of sensitivity tests. The assessment of goodness of fit of all these tests relies on the post-test match, in which a comparison was made between the modelled calculated head values and the measured data. In doing so, the model concept was progressively and iteratively updated and modified until there was little difference between the modelled freshwater head profiles and the values measured from monitoring wells.

4 THREE-LAYER MODEL

4.1 Concept addressed

The aim of the Three-layer model is to test the basic credibility of the conceptual model with respect to head and flow under the most simplified assumptions. This model has three different types of material:
a) The upper part, the Sherwood Sandstone Group, with high permeability, was treated as a single-layer aquifer
b) The least permeable Permian, including, the St. Bees Evaporites, the St. Bees Shale and the Brockram was taken as a layer of aquiclude.
c) The Basement and Hill area, with its moderate low permeability were taken as an aquitard. The cross section is shown in Figure 4-3(a).

Offsets produced by faulting are included in this model, but there is no attempt in this model to consider any intrinsic petrophysical effects associated with fault zones.

4.2 Input parameter values

In the base model of this set of simulations, the Sherwood Sandstone Group was assumed to be homogenous and its hydraulic conductivity was set to 20 mD, which is the same as the measured value for the Calder Sandstone in the field. The aquiclude in the middle was assigned a value of 0.01 mD and the aquitard at the bottom was set to 0.1 mD. The porosity used was the measured median value.

4.3 Sensitivity results

To obtain a high degree of confidence in a model and its results, comparison of the models and system's input-output is required. The model and real systems behavior data are plotted on graphs for various sets of experimental conditions to determine if the models output behavior has sufficient accuracy for its intended purpose. For a given distinctive fluid type and for a constant head, the groundwater flow is solely determined by the hydraulic conductivity of the rocks. As a starting point of each sensitivity test, I compared the calculated heads, as affected by changes in hydraulic conductivity of the three materials, and those measured in the deep borehole 3 (Figure 4-4). It was found that the modelled fresh water heads are far below the measured values.

The model is particularly sensitive to changes in permeability of the bottom layer and mid layer, indicating that the low-permeability basement is an important part in this groundwater flow system. When the permeability of the aquifer was increased, the modelled water head became higher but still well below the measured ones. Changes in the permeability of the mid layer are correlated with changing the modelled head. Conversely, changes in the basement permeability are inversely correlated with the modelled head. That implies that the basement rock should be less permeable than it was assumed in the base case.

The effect of anisotropy was tentatively tested at this stage of modelling. The results indicate that only the top aquifer in three-layer model exhibits an effect related to permeability anisotropy. The result is plotted in Figure 4-5.

4.4 Flow pattern

The groundwater flow pattern can be depicted through plots of average linear velocity (Figure 4-6) and by streamline contours (Figure 4-7). In the three-layer model, the flow occurs dominantly in the top aquifer, and the basement is a zone of almost no flux. From the streamline contours it can be seen that the groundwater in the hill area flows towards the west, and groundwater in the repository zone is recharged from the hills. It is of interest to note that there is a natural flow division boundary between the Sellafield area and the Lake District area, about 19 km to the east of the coast (Figure 4-7). This boundary implies that the total possible recharge from the east to the repository area, has been included in the regional model and the eastern boundary of the model is far beyond the recharge limit. Due to the identification of brine water in the west, a density driven circulation is established between the extremely dense brine waters in the west and those of the saline waters in the hills area.

The flow pattern is considerably affected in response to changes in the permeability of the bottom layer. More groundwater flow occurs in the basement when its permeability was increased to be equal to that of the aquiclude (Figure 4-8).

4.5 Temperature distribution

Temperature has an effect on groundwater properties, and rapid flows can alter the temperature distribution. Figure 4-9 illustrates the temperature distribution calculated in the model. The contour map shows that the temperature contour lines follow the topography owing to the extremely slow groundwater flow and the insignificant heat transport resulting from it. However, the temperature contour lines changed greatly once the permeability of the bottom rock was increased to cause convection fluid flow in it, with the consequences of heat transportation (Figure 4-10).

4.6 Summary

The first step of the modelling is to use the three-layer model, which reveals some of the basic nature of groundwater flow in West Cumbria. There is a natural flow divide boundary existing in this regional model, lying between the Sellafield area and the Lake District area, about 19 km in the east from the coast. It implies that the total possible recharge from east of the repository area has been included in the regional model. In spite of that, the simple model is too simple to reproduce the actual groundwater flow, particularly the basement flow. The model still indicates that the low permeability basement plays an important part in regional flow, even though it is of very low permeability.

5 SEVEN-LAYER MODEL

5.1 Concepts addressed

The next step in the modelling is to better account for the range of materials in the area. The objective of a Seven-layer model is to identify the hydrogeological influences controlling groundwater flow at Sellafield. In this model, these materials are: Calder Sandstone; St. Bees Sandstone; Permian; Carboniferous Limestone; Borrowdale Volcanic Group; Skiddaw Group and Granite. The faults are not involved at this stage except to account for their offsets. The cross section is shown in Figure 4-3(b). For the Seven-layer Model, measured head in two deep boreholes provides constraints: Borehole 2 in the PRZ area and Borehole 3 located at the coastline.

5.2 Input parameters

The base-case parameter values used in the Seven-layer model were derived from the mean values obtained from field measurements (Table 4.1). The permeability of Calder Sandstone was set to 200 mD, that of St. Bees Sandstone was 20 mD, 0.004 mD was used for the Permian, Carboniferous was input 2 mD, the BVG was set at 0.002 mD, the permeability of the Granite and the Skiddaw Group was assumed to be 0.004 mD and 0.001 mD respectively.

5.3 Sensitivity analysis

5.3.1 *Permeability*

In this series of tests, the permeability of each hydrostratigraphic unit is varied in turn, i.e., changing each individual permeability of unit and predicting corresponding groundwater heads. The resulting calculated heads are compared with heads measured in the two boreholes: Borehole 3 and Borehole 2. The matches are analysed in the graphs in which the head is plotted against the depth. All the results are illustrated from Figure 4-11 to Figure 4-17.

The sensitivity test in the Seven-layer model shows great response of the groundwater heads to the changes of permeability. All the test results are varied from unit to unit, and from borehole to borehole in the single unit. Among them, the Calder Sandstone, the BVG, and the Skiddaw Group exhibit a great deal of response to the changes of permeability.

In a series of simulations, the permeability of the Calder Sandstone was varied from 0.2 mD to 200 mD. The corresponding computed groundwater head was compared with the real measured values (Figure 4-11). The modelled head is sensitive to changes of permeability. The computed heads approach the measured ones, in both Borehole 3 and Borehole 2, when the permeability of the Calder Sandstone is increased from 0.2 mD to 200 mD. The head in Borehole 3 is more sensitive to changes in the permeability of the Calder Sandstone; this is reasonable because there are over 500 m of Calder Sandstone in Borehole 3 and none of it in Borehole 2. The modelled groundwater head matched much better when the permeability of the Calder Sandstone was between 20 mD and 200 mD, which is within the range of median field values.

Nevertheless, sensitivity tests show that the St. Bees Sandstone has little effect on the energy of the flow system (Figure 4-12) when the permeabilities of the St Bees Sandstone were tested from 0.2 mD to 200 mD. Only in Borehole 3 was the upper region of the modelled head profile noticeably closer to the measured values at a permeability between 2 mD and 20 mD.

The effect of changes in the permeability of the Permian was evaluated by varying its value between 0.0004 mD and 0.4 mD (Figure 4-13). At the position of Borehole 3, we can see that the calculated head is not sensitive to the changes of permeability. In contrast, the calculated head is rather sensitive in Borehole 2. When the permeability increased from 0.0004 mD to 0.4 mD, the calculated head changed from an excessively high value, to values closer to those measured ones.

The permeability of Carboniferous Limestone was varied from 0.002 mD to 20 mD (Figure 4-14). Changes in permeability of Carboniferous Limestone have little impact on the computed freshwater head except at the bottom of Borehole 3, where the calculated head approaches the measured head when the permeability is in excess of 0.2 mD. Since Carboniferous Limestone is not present in BH2, there is little effect noted in this location.

The sensitivity test of permeability in the BVG was analysed by varying its values from 0.0002 mD to 0.2 mD. Figure 4-15 illustrates that calculated groundwater head was very sensitive to changes in the permeability of the BVG, in particular in Borehole 2 where the PRZ was to be located. In contrast to the case with Carboniferous Limestone, the modelled head in Borehole 3 declines when the BVG permeability exceeds 0.02 mD. In borehole 2, the computed head is very sensitive to changes in the permeability; hence, the computed head is much higher than the measured head when the permeability is below 0.002 mD.

The permeability of the Skiddaw Group was varied from 0.0004 mD to 0.4 mD (Figure 4-16). It is surprising that the modelled head in Borehole 2 is very sensitive to changes in the permeability of the Skiddaw Group, even though it is 4 km deep, beneath the Borrowdale Volcanic Group. This result suggests that the best fit value is between 0.0004 and 0.004 mD.

The granite permeability has little effect on the groundwater flow system at Sellafield area when its values varied from 0.0001 mD to 0.1 mD (Figure 4-17), because it is far from the PRZ area.

5.3.2 *Anisotropy*

Anisotropy was revealed in the core samples, with the horizontal conductivity being 0 - 2 orders of magnitude more than the vertical conductivity (see Table 4-1). The anisotropy of all materials in this region was investigated as was the sensitivity of permeability, using the ratio of horizontal to vertical hydraulic conductivity (k_h/k_v), which varied from 0.0001 to 1. The results are shown in Figure 4-18 to Figure 4-24. The anisotropy tests indicate that the water head is sensitive to the changes of the ratios of: sandstone, BVG and Skiddaw Group.

When testing the anisotropy of the Calder Sandstone, the predicted heads were going down below the measured value while increasing the ratio from 0.1 to 100. The test results suggested that the best fit anisotropic ratio (k_h/k_v) of hydraulic conductivity of the Calder Sandstone is between 1 and 10. Likewise, the test of St Bees Sandstone showed the same result and its best fit ratio is around 10. The anisotropy sensitivity tests illustrate that the Sandstone Group is only slightly anisotropic.

Owing to the small thinness of the Permian and Limestone at the monitoring Borehole site, the sensitivity test of anisotropy is not very significant. Even so the test results still show the best fit ratio of Permian is between 10 and 100, which exhibits strongly anisotropic characters.

Based on comparing values of permeability on core samples to values derived from borehole tests, it was concluded that the groundwater flow in the BVG is overwhelmingly controlled by connected network of larger open fractures rather than the rock matrix with microfractures (NIREX, 1993a). Accordingly the BVG should be anisotropic rather than isotropic. The anisotropy tests indicate that the best fit ratio of the BVG and Skiddaw Group is between 0.1 and 1.

5.4 Groundwater flow pattern and flow rate

To characterise and quantify the groundwater flow system, the average linear velocity of the groundwater was calculated for each simulation. The velocity for the best fit Seven-layer Model is plotted in Figure 4-25. Most of the flow directions travel towards the shallow sandstones, especially the Calder Sandstone that forms the main aquifer in this area. The maximum flow rate in this simulation is 1000 m/yr and occurs in the Calder Sandstone. In contrast, the flow rate in the BVG around the PRZ is very slow, less than 0.1m/yr.

As was discussed before, the groundwater flow is fundamentally controlled by the groundwater head gradient and the permeability of the medium. Thus the groundwater flow pattern varied considerably during the sensitivity tests. From Darcy's law we know that the flow rate can have a wide range when water head is kept the same while the hydraulic conductivity changes. In other words, the water velocity could vary greatly even though similar groundwater heads were produced repeatedly. Hence it is very important to examine the flow rate while matching the heads with measured ones. In this study, the emphasis was placed on investigating the flow rate in the volume of the PRZ and its surrounding area. The most obvious effect on the groundwater flow near the PRZ comes from the hydraulic properties of the BVG and the Skiddaw Group.

When the permeability of the sandstone group is increased, the groundwater flow is focused in it, and is much more rapid, but there is little effect on flow rate in the BVG. There are no detectable influences from changes of permeability of the Permian and the Limestone on the flow rate in the Sandstones and Basement. The groundwater flow rate in the BVG is most clearly controlled by its own permeability. When the permeability of the BVG is increased by two orders of magnitude, its flow rate is one order of magnitude higher. However there is no effect on the flow rate of the upper units. It is of interest to note that the flow rate in the BVG is also dependent on the hydraulic properties of the Skiddaw Group underneath. For instance, if the permeability of the Skiddaw Group was enhanced two orders of magnitude (say to 0.1 mD), the flow rate of the BVG increased by one order of magnitude as well (to about 10 m/yr). This effect was also deduced by Haszeldine and McKeown (1999), using a much smaller local model. It was also noticed that not only did the flow rate in the BVG go up, but also the flow rate in the Sandstone Group was raised when increasing the permeability of the Skiddaw Group. The granite plays no part in controlling the flow rate in the PRZ during these simulations.

The groundwater flow paths can be seen in the contour map of streamlines (Figure 4-26). In the Sellafield area, the groundwater is recharged from precipitation on land and hill areas, going downwards driven by topography, then being forced up into the BVG and discharging to the upper aquifer. As an interface of brine water and fresh water exists offshore, there is a local circulation around this area resulting from the density variation (Figure 4-27). Compared with the Three-Layer Model, the local convection was smaller in the Seven-Layer Model. Details of the factors controlling streamlines will be discussed in the next section in the comprehensive model.

5.5 Temperature distribution

The calculated temperature distribution is affected by variations of the groundwater flow pattern that result from changes in the permeability. The base case temperature distribution is presented in Figure 4-28. The Seven-Layer model temperature distribution is similar to that of the Three-Layer Model, but contours are smooth in the coastal area because there is less local circulation in the Seven-Layer model. In general, the higher flux of fluid, the more capacity for heat exchange. When groundwater flow is across the temperature contours, there is the potential for disturbing the temperature patterns. The most significant effect on the temperature distribution occurs within the basement, a more permeable basement (one order magnitude higher permeability than the base case) results in more heat exchange (Figure 4-29).

5.6 Summary

The calibration model via sensitivity analysis for the Seven-layer model described above illustrates that the calculated heads were very sensitive to the changes of permeability. It also confirmed the basic relationship between the hydraulic properties of the rocks and the head distribution. In particular, the hydraulic conductivity of the Calder Sandstone controls the shallow groundwater flow and heads, while the St Bees Sandstone has a lesser effect. The deep groundwater head is dependent on the permeability of the BVG and the Skiddaw Group. Strikingly, changes in the hydraulic properties of underlying units have little effect on the groundwater head in overlying units. Not only did the groundwater head distribution change when the permeability was varied, but the flow rates also changed as well. The best fit hydraulic conductivities are presented in Table 4.2 and the results of the calculated heads from these best-fit permeabilities are plotted in Figure 4-30. These calculated heads are very close to the ones measured in the field. This gives confidence that an accurate simulation is being achieved.

The groundwater head profile in Borehole 2 where the PRZ is located can be reproduced very well using the Seven-Layer Model. By contrast, Heathcote *et al* (1996) attempted to reproduce the groundwater head in Borehole 2 in their models. They had to increase the salinity to a value well above the observed salinity in order to obtain this match. However, the groundwater head profile in Borehole 2 was well reproduced in my regional model without any change in observed in-situ salinity.

In addition to affecting the groundwater head distribution, the hydraulic properties also have a significant effect on the flow and the temperature distribution. Even though parameters derived from tests are not unique, the simulations suggest that the groundwater head pattern also depends on the ratio of permeability anisotropy of the materials.

There is still a slight difference between modelled head in this Seven-layer Model and measured values in Borehole 3, in particular at the bottom of this borehole. It was unable to find a combination of hydraulic parameters that simultaneously reproduced the head profiles for both Borehole 2 and Borehole 3. This result suggests that additional factors need to be included in the models.

6 COMPREHENSIVE MODEL

6.1 Introduction

The accuracy of modelling was assessed by comparison between the calculated results and measured values in situ. Although the Seven-layer model heads match the two borehole data, which are three kilometers apart, this does not necessarily mean that the modelled heads can also match the measured heads in other boreholes in between. It was found that the best fit of results for Borehole 2 and 3 in a Seven-layer Model did not fit with measured values in borehole 10A. The comparison between computed heads and measured ones was made in Borehole 10A, and can be seen in Figure 4-31. So a further, more complicated model needs be constructed to represent the real hydrogeological system.

The aim of this comprehensive model was to try and reproduce the groundwater head accurately using all the currently available data, since the previous simpler models did not satisfactorily match the real systems. All the materials that were discovered in the area will be involved in the comprehensive model, in particular, the Glacial Drift and Fault Zones. Nine types of materials are included in this model: Drift; Calder Sandstone; St. Bees Sandstone; Permian; Carboniferous Limestone; Borrowdale Volcanic Group; Skiddaw Group; Granite; fault zones. The cross section map is given in Figure 4-3(c). The mesh used in this model was the same as before in the Seven-layer Model. To fully understand the impact of stratigraphy on the groundwater flow, three boreholes at different locations were introduced in the test, to match measured data, trying to enhance confidence in the model. These boreholes from west to east are Borehole 3, Borehole 10A and Borehole 2.

6.1.1 *Hydraulic properties of faults and fractures at Sellafield*

Groundwater flow through and around the Potential Repository Zone at Sellafield is dominantly in fractures (Michie, 1996). Characterization of the hydrogeological system is therefore directly related to the determination of controls of fracture flow. Faults and fault zones were spotted throughout drilling investigation at Sellafield, and their hydrogeological properties were tested during drilling or post drilling (NIREX, 1993d). The hydrogeological information on faults and minor lithologies consists of inflow points from Full Section Tests (FSTs) and hydraulic conductivity and head data from EPMs(NIREX, 1993d). Some results from DETs and PDDETs are also available. From the NIREX investigation, faults (main plus minor) account for 36% of the flow zone structures (NIREX, 1993d). These tests reveal that the fracture families in any particular structural setting were not favoured as flow structures. In Borehole 2, only six of 18 fracture families appear to be closely related to faults, but the larger flow zones tend to be associated with fracture families and minor faults. Only one of the two largest flows is associated with a single fracture (Borehole 2). Some points can be drawn from the statistics from NIREX (NIREX, 1993d):

(a) Nearly half the flowing features are associated with NE-dipping structures, the remaining larger flows tend to link with structure families and minor faults oriented NNW-SSE.

(b) Flow occurs through the fracture system, but fracture envelopes to faults are not particularly associated with flow zones.

(c) On average, 50m test zones which contain logged faults are more transmissive, by about $1^1/_2$ orders of magnitude than those without.

(d) There is no enhanced transmissivity where the major faults intersect Boreholes 2, 4 and 5.

From the above discussion we can see that the flow does occur through the fracture system, but is not necessarily particularly associated with fault zones. This implies that fault zones would not simply treated as uniformly permeable layer.

Fault representation and scaling in flow models are examined in this model with respect to fault zone properties. Representation of faults conflates the effects of four factors — fault zone thickness and permeability, grid-block size and matrix cell permeability. To quantify the groundwater flow in these faults and fractures, and their effects in the regional flow system as well, I used three columns of mesh to mimic the conceptualised fault (fractured) zone in this comprehensive model, each column was ten meters wide.

6.2 Input parameters

The parameter values in the base case comprehensive model were based on the median values obtained from field measurements and previous modelling tests. The hydrogeological units in this model are the Drift, the Calder Sandstone, the St. Bees Sandstone, the Permian , the Carboniferous, the BVG, the Granite, the Skiddaw Group, and faults. The permeability of Drift was assigned as 20 mD, Calder Sandstone was set to 20 mD, that of the St. Bees Sandstone was 20 mD, the Permian was 0.004 mD, the Carboniferous was input as 2 mD, the BVG was set 0.002 mD, the Skiddaw Group and Granite were assumed to 0.002 mD and 0.0004 mD, the faults were assigned between 0.01 mD and 20 mD.

6.3 Sensitivity analysis

In the sensitivity analysis testing of this model, more borehole data were introduced to analyse the accuracy of simulations of the real system. As seven of these nine materials had been tested before, the sensitivity testing of the comprehensive model was focused on the other two materials, Drift and Faults, the Drift was assumed as isotropic. During this test, three deep borehole data, Borehole 3 at the coastline, Borehole 2 in the PRZ area, and Borehole 10A in between, were used to compare with the computed water head and to test the sensitivity of the parameters. The results of the tests were assessed by plotting computed head and comparing with those measured at the same depth.

In the series of sensitivity tests, the permeability of Drift varied from 0.2 mD to 200 mD and the results are given in Figure 4-32. The sensitivity test in the comprehensive model suggested that the modelled water head was also moderately sensitive to the changes in the permeability of the Drift, with most effect for the upper heads. The groundwater head was raised when the permeability of the Drift was decreased in the model. The reason for this might be the confined effect of the system when lowering the conductivity of the Drift.

A sensitivity test of permeability on faults was investigated through two steps. Firstly, the fault was treated as a single medium, i.e., it was uniform from bottom to top of the cross section. But this simplifying assumption proved unrealistic after no good match of the computation was obtained. That means the hydraulic properties of faults vary between units. Secondly, under such circumstances, the fault was assigned varied parameters that depend on its surrounding lithology. It was found that this case could match the monitoring data very well. In doing the sensitivity tests, the modelled head was also very sensitive to changes in the hydraulic properties of faults, when varying the permeability from values lower than surrounding rocks to values higher than surrounding rocks. The results of sensitivity tests of permeability on faults in the BVG are shown in Figure 4-33. Basically, when the fault or fracture zone is more permeable than its surrounding rocks, the highest anisotropy value should be vertical. The trend of the response is reversely correlated to permeability: the lower permeability, the higher groundwater head was obtained. In contrast to the Drift, the groundwater head responded greatly to the changes of permeability only in locations below the Permian. That is reasonable because the hydraulic properties of the BVG are overwhelmingly controlled by the fractures and faults in it. The anisotropy of the fault was also tested by varying the ratio of horizontal permeability to vertical permeability from 0.01 to 10 mD. The results were plotted in Figure 4-34. and the best fit ratio of anisotropy of faults stands between 0.1 and 1. The modelled permeability testing of faults shows the fault zones are only slightly more permeable than the surrounding rocks. This implies that the connections of these fractures are very limited, which coincides with field observations and core log measurements (NIREX, 1993b).

More complexity resulted from introducing more borehole data to match the modelled values, because the response of the sensitivity tests varied from borehole to borehole. For instance, when using the best fit parameters derived from the Seven -layer Model, the results of simulations matched boreholes 2 and 3. However, groundwater heads did not fit the Comprehensive Model when comparing the borehole 10A water heads measured in-situ. As a result of this, all the hydraulic properties of those materials in Sellafield were retested to try and match the three deep boreholes' data. The result of this sensitivity test is not unique, particularly in this complicated model. I tested all the possible combinations of changes of these parameters and obtained the best-fit sets of parameters which best match the real groundwater head in all the three boreholes, Borehole 3, Borehole 10A and Borehole 2. These results are given in Table 4.2. The modelled water heads are very close to the measured values in the comprehensive model, which is illustrated in Figure 4-35.

It is of importance to note that the parameters used in the elements of individual rock units are identical, because we tried to simulate the regional groundwater flow system in the general case, which is vital in regional modelling. It is most useful when the general case actually works, in spite of constraints from limited borehole data in situ. Then we can say that the assumptions are basically correct and reliable. In these tests we tried to reproduce the basic features of the groundwater flow system at Sellafield using median parameters. For some exceptional data this does not work. For example, from EPM test in situ, due to the fracture flowing zone, there were some extremely low groundwater heads in the BVG at Borehole 2. These exceptionally low heads can be modelled separately by assigning specific high permeability value in the local mesh.

Since the most significant of the responses of groundwater heads to the sensitivity tests occurred in Borehole 2, it is critical to obtain matches of the measured heads in Borehole 2. The NIREX two-dimension vertical cross section model used only two boreholes data to match with their modelled water head, in Borehole 3 and Borehole 2. Nevertheless, NIREX models were not able to match the head in Borehole 2. In this sense the comprehensive model of this thesis might be a more reliable model, since it successfully reproduced the three borehole head measurements at the same time and so more precisely represents the actual groundwater flow system.

6.4 Groundwater flow pattern and flow rate

The groundwater flow pattern and flow rate in the area were calculated when the best fit parameters were obtained through sensitivity tests. From the comprehensive model, the groundwater flow was focused in the sandstone aquifer with flow rates between 10 m/yr and 100 m/yr. Meanwhile, the flow rate in Faults varied from 0.01 m/yr to 1 m/yr. The groundwater velocity in the eastern part of the basement was higher than that of 3 or 7 layer models, about 1 m/yr. The flow rate in the PRZ was between 0.1 m/yr and 1 m/yr, and it was 0.1 m/yr in the Skiddaw Group. One of these simulated results was plotted in Figure 4-36.

The flow pattern and flow path can easily be seen in the flow rate graph (Figure 4-36) and streamline contour map (Figure 4-37) respectively. Both maps clearly show that the groundwater percolates through the Granite and BVG after being recharged from precipitation, and it diverts into west and east flows. The west part goes deeply downwards and then upwards into sediments, forming recharge of groundwater at the Sellafield PRZ, then flows towards the west coast. This suggests that the groundwater in the potential repository zone is recharged both from the deep basement and by a lateral flow from the east. Most of the fresh water goes directly into the superficial aquifer after precipitation, forming the freshwater regime, and discharges to the west coast. For the East Irish Sea Brine water Regime, waters are almost static with flow rates less than 0.01 m/yr driven by basinal forces. All these flow systems agree with the conceptual model. It should be noted that there is still groundwater flow occurring offshore above the brine water regime driven by topography from the coast towards the center of Irish Sea with a flow rate about 1 m/yr. We call this the Shallow Water Regime.

There is not much influence on the flow pattern when changing the hydraulic properties of the Glacial drift and faults, this might due to the their limited local distribution. The difference between the Seven-layer Model and the Comprehensive model in flow pattern is that the convection caused by the interface between saline water and brine water becomes smaller. There are also more stream lines existing in the basement in the Comprehensive model, this means more flux (convection) occurred in this model.

6.5 Temperature distribution

The heat transport calculated in this model was illustrated using a temperature contour map (Figure 4-38). Because of more water flux in the basement from the Comprehensive Model, the temperature contour lines fluctuate more than ever before. It seems that the contour lines follow the boundary between the aquifer of the sandstone and the aquitard of the Permian. It illustrates that the groundwater flow controls the heat transportation in this area.

6.6 Conclusion

The hydraulic properties of all the units in west Cumbria were investigated using a comprehensive model, which compared between modelled groundwater head files and measured heads from investigation boreholes. Some conclusions can be drawn from the Comprehensive Model:

a) All the types of rocks discovered at Sellafield play an important part in affecting groundwater flow in this area. The best fit parameters vary from borehole to borehole, the more borehole data used, the more difficult it is to match all of these.

b) The groundwater heads measured in three deep boreholes along this cross section can be accurately reproduced using the Comprehensive model.

c) The groundwater heads are controlled by the medium's hydraulic properties. The upper layer permeability change will affect groundwater head in the underlying materials, but not vice versa. The deep groundwater head is critically dependent on the permeability of both the BVG and Skiddaw Group. Changes of hydraulic properties of these underlying units have little effect on groundwater head in overlying units but greatly affect the flow rate.

d) The low permeability basement (Skiddaw Group) plays a key role in controlling the deep underground water head, but it has no effect on the groundwater heads of the upper layers. It is vitally important in accurate regional modelling. However low permeability basement is often neglected in conventional hydrogeological modelling.

e) Groundwater flow in low permeability basement rocks is controlled by the fractures in them. The connection of fractures in faults and the fracture zones is very limited and they are not very conductive through the modelling tests. This is consistent with the measurements from field investigations.

f) The study of groundwater flow modelling shows the groundwater flow system at Sellafield is recharged by precipitation at the surface of the land and hills. A natural groundwater boundary exists in the subsurface twenty kilometers east from the coast, where groundwater percolates into and diverts into either west or east flows. This meteoric water flows into the deep underground and rises up westwards towards the coast where it meets brine water. Groundwater discharges to the west after entering the aquifer of the Sandstone group and merges into the East Irish Basin.

g) Temperature distribution depends on the heat transportation resulting from the fluid flow system.

7 SUMMARY

The groundwater flow at Sellafield was simulated progressively from a simple Three-layer model to a very complicated Comprehensive model. During these modelling steps, the modelled water head approaches progressively to the measured values from the simple model to the comprehensive one. This implies that the concept of these models is close to the real system.

The first stage of modelling was to use a three-layer Model, to test the credibility of assumptions in a conceptual model with respect to head and flow in a most simplified system. The hydraulic properties of the materials were tentatively tested using only groundwater heads measured in deep Borehole 3 at this stage of modelling. Although this model is too simple to represent the real system, it reveals some basic features of the regional groundwater flow system.

The second stage of modelling was to use a Seven-layer Model, incorporating most of the stratigraphy, to investigate the lithostratigraphical effects on the groundwater flow. The results of the tests were analysed using two boreholes' data, Borehole 3 and Borehole 2, three kilometers apart. Assessment of those modelled groundwater heads was carried out by plotting heads against depth. The sensitivity tests in this Seven-layer model indicate that the groundwater head is significantly sensitive to the changes of hydraulic parameters, which vary from layer to layer or from borehole to borehole even within the same stratigraphy. Among them, the Calder Sandstone, the BVG, and the Skiddaw Group produce a great deal of response to the changes of permeability. All the monitoring heads in Borehole 2 and Borehole 3 used in assessment can be matched very well in this Seven-layer Model.

The most striking point is that the groundwater head can be successfully reproduced using this regional model. This is especially so for the heads in Borehole 2, in which heads modelled by others (Heathcote *et al*, 1996) were far below the measured values in-situ. The reason for this might be that the low permeability Skiddaw Slate basement, which has previously been neglected, was explicitly considered in my regional model. This deep rock unit plays an important part in the regional model and in particular in the deep groundwater flow.

The response of modelled groundwater head to the tests of hydraulic properties varied from borehole to borehole. More complexity resulted from introducing more borehole data to match the modelled values. Therefore, the three deep boreholes' data were used to test the credibility of the model, they are Borehole 3, Borehole 2, and Borehole 10A. Generally speaking, the more measured boreholes' head data are introduced to be matched, the more difficulties are encountered in trying to match them all at the same time. This is because the parameters for the model matching one borehole do not necessarily suit the others. It should be appreciated that all the heads measured in these boreholes can be matched better between calculated and measured values after introducing the Comprehensive Model, in which all the materials discovered at Sellafield were involved in the model, explicitly including Drift, and Fault Zones.

From the calculation of heat transport using these models, it is indicated that the heat transportation is dependent on the fluid flow system in this area.

The study of groundwater flow modelling indicates the groundwater flow system modelled is consistent with the conceptual model. This suggests that the groundwaters were recharged from precipitation in the east hill areas, percolating through the Granite and BVG, going down and then rising west upwards into sediments, finally flowing west towards the coast. This still shows that the groundwater in the repository zone is recharged both from the basement and by lateral flow from an east boundary. Most of the fresh water goes directly into the superficial aquifer after precipitation, and discharges west to the coast, forming the Coastal Shallow Water Regime. There is also groundwater flow existing above the brine water regime driven by topography from the coast towards the central Irish Sea with a flow rate of about 1 m/yr. Those brine waters in the East Irish Sea Basin Regime are almost static.

From the sensitivity analysis of permeability and anisotropy we can conclude that the comprehensive model can accurately reproduce the measured heads. The parameters fed into the model are still in accordance with the values measured in the field. In spite of this, there is still a slight difference in the upper part of borehole 3 between modelled and measured heads. In addition, to match the water head in Borehole 3, the permeability of the St. Bees Sandstone needs to be higher than the Calder Sandstone, which is contradictory to the field measurements. Consequently, there might be some improvements still possible in these models.

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		Calder Sandstone	**St Bees Sandstone**	**Permian**	**Carbonif-erous**	**BVG**
Field K (log ms^{-1})	Min	-7.5	-10.1	-12.4	-8.6	-13.1
	Med	-7.0	-7.6	-9.2	-7.3	-10.0
	Max	-4.8	-5.0	-5.0	-5.1	-6.0
Core Kh (log ms^{-1})	Min	-8.7	-10.4	-11.0	-10.7	-11.0
	Med	-6.3	-7.7	-9.7	-10.4	-10.5
	Max	-5.2	-5.5	-7.0	-9.0	-7.1
Core Kv (log ms^{-1})	Min	-8.7	-10.5	-11.0	-10.7	-11.0
	Med	-6.7	-8.3	-10.2	-10.5	-10.4
	Max	-5.2	-5.6	-7.0	-8.5	-7.7
Core Porosity (%)	Min	13.4	1.5	0.6	0.2	0.1
	Med	19.5	11.6	2.9	1.2	0.8
	Max	26.3	21.6	11.4	5.9	7.2

Table 4.1 Hydrogeological properties of units (from NIREX report 524)

Hydraulic conductivity (m/yr)	**Drift**	**Calder Sandstone**	**St Bees Sandstone**	**Permian**	**arboniferous Limestone**	**BVG**
NIREX Value (Median Field value)	180	3	0.93	0.018	1.5	0.003
Seven-layer Model Set 1	60	30	80	0.006	6	0.18
Seven-layer Model Set 2	10	6	8	0.0006	0.6	0.012
Comprehensive Model	10	3	0.3	0.0012	1.24	0.15

Table 4.2 The best fit of hydraulic conductivity values in Seven-layer and Comprehensive Models

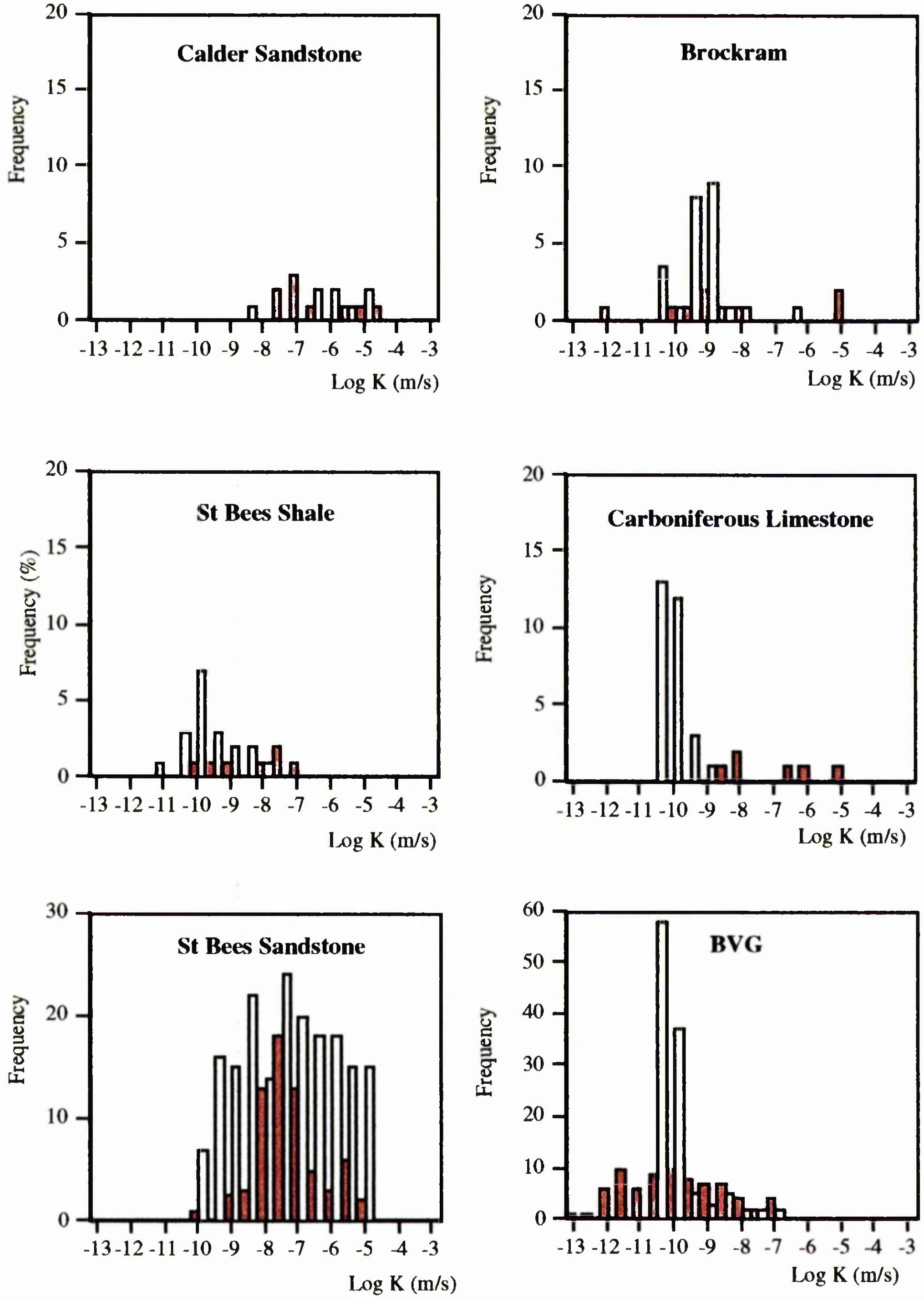


Figure 4-1 Hydraulic conductivities measured in the units

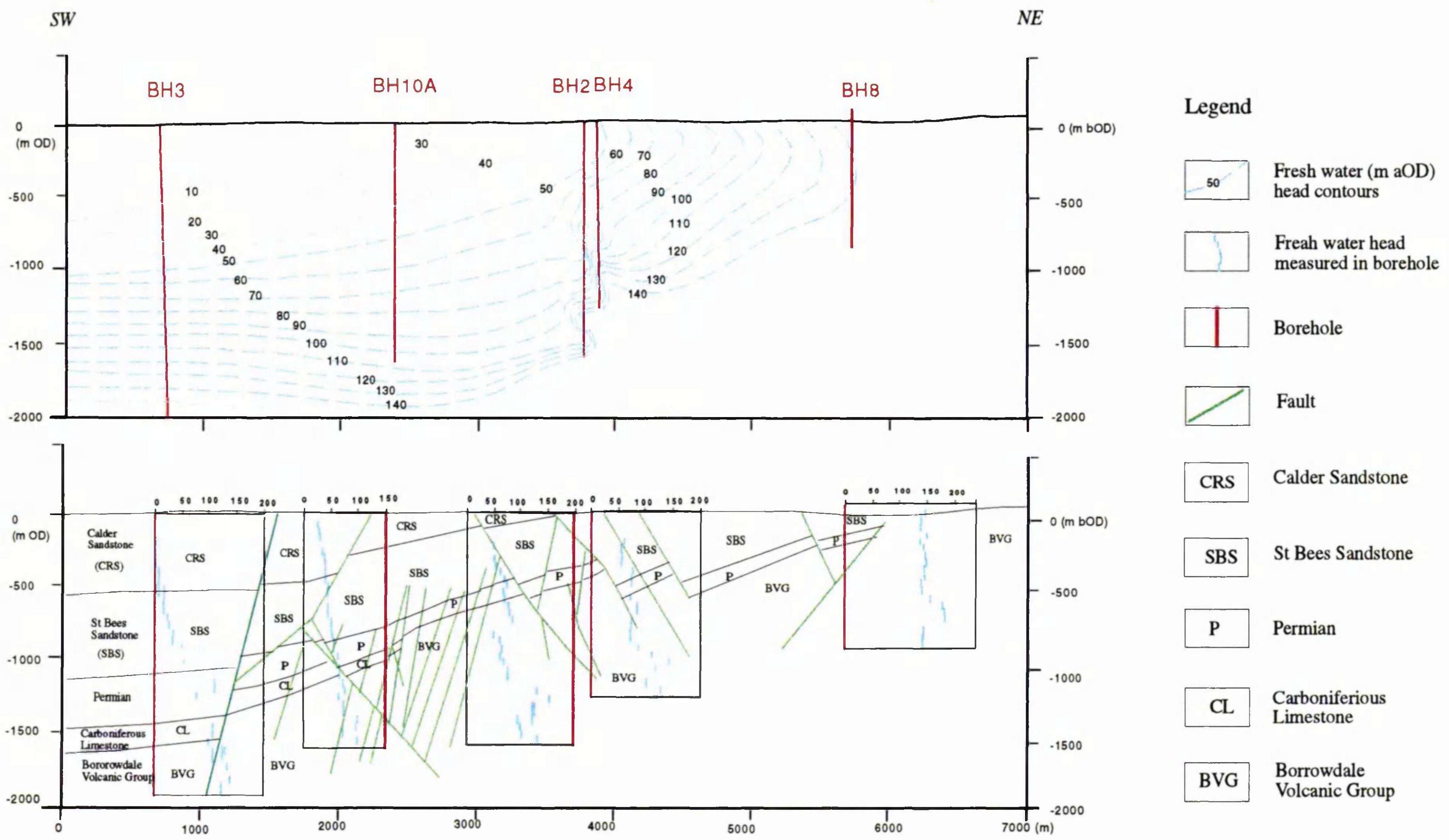
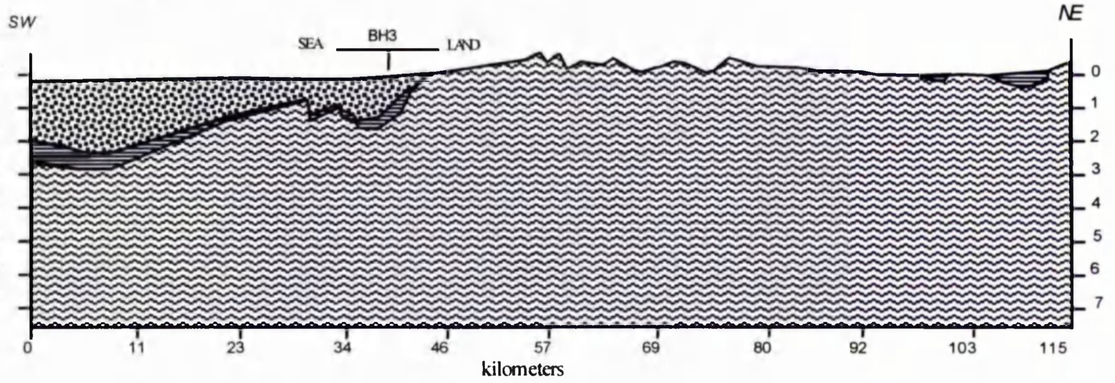
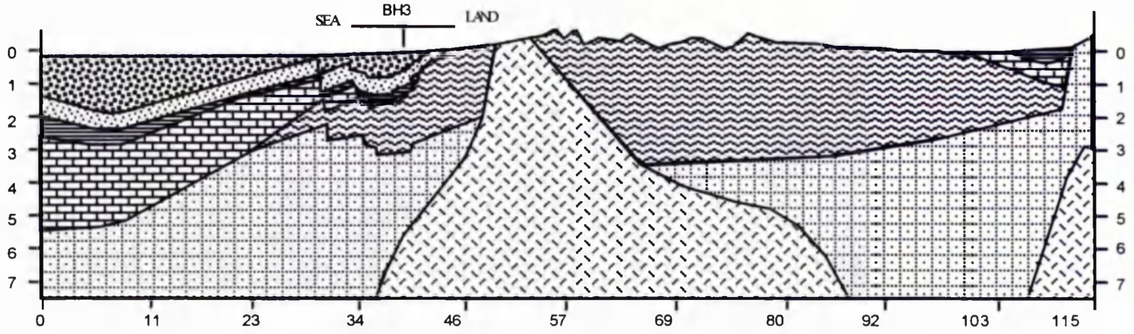


Figure 4-2 The local groundwater head and contours distribution along the cross section (from NIREX, 1993b)

(a) **THREE-LAYER MODEL CROSS SECTION**



(b) **SEVEN-LAYER MODEL CROSS SECTION**



(C) **COMPREHENSIVE MODEL CROSS SECTION**

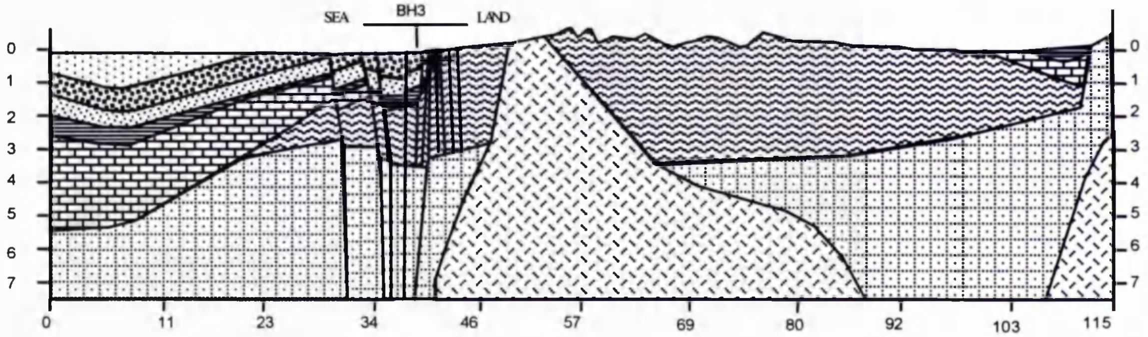
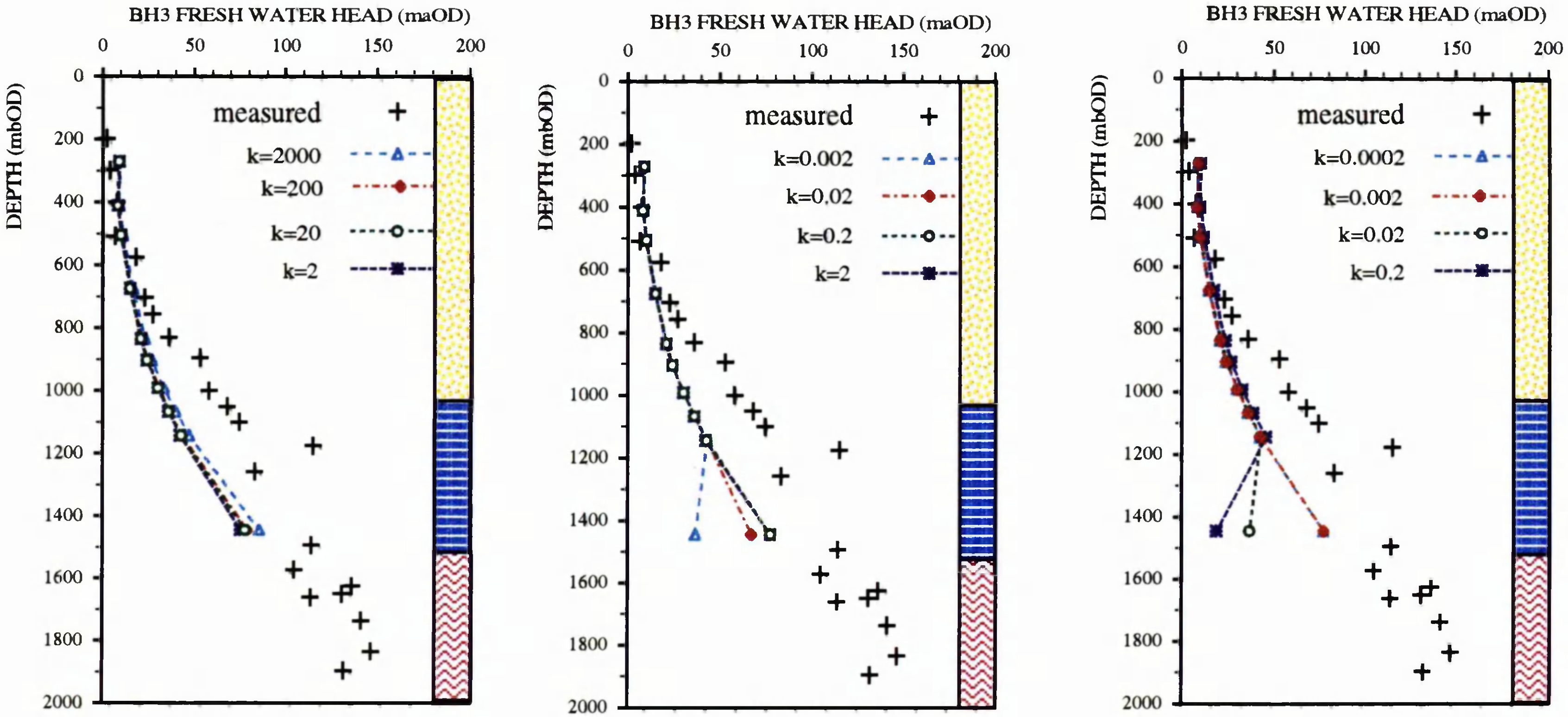


Figure 4-3 Cross sections and materials used in various stages of the models



Top Layer (Aquifer)

Mid Layer (Aquitard)

Bottom Layer (Aquiclude)

Figure 4-4 Sensitivity test of Permeability in the Three-layer Model

The permeability were tested within four magnitude ranges, but all the modelled heads are well below the measured ones.

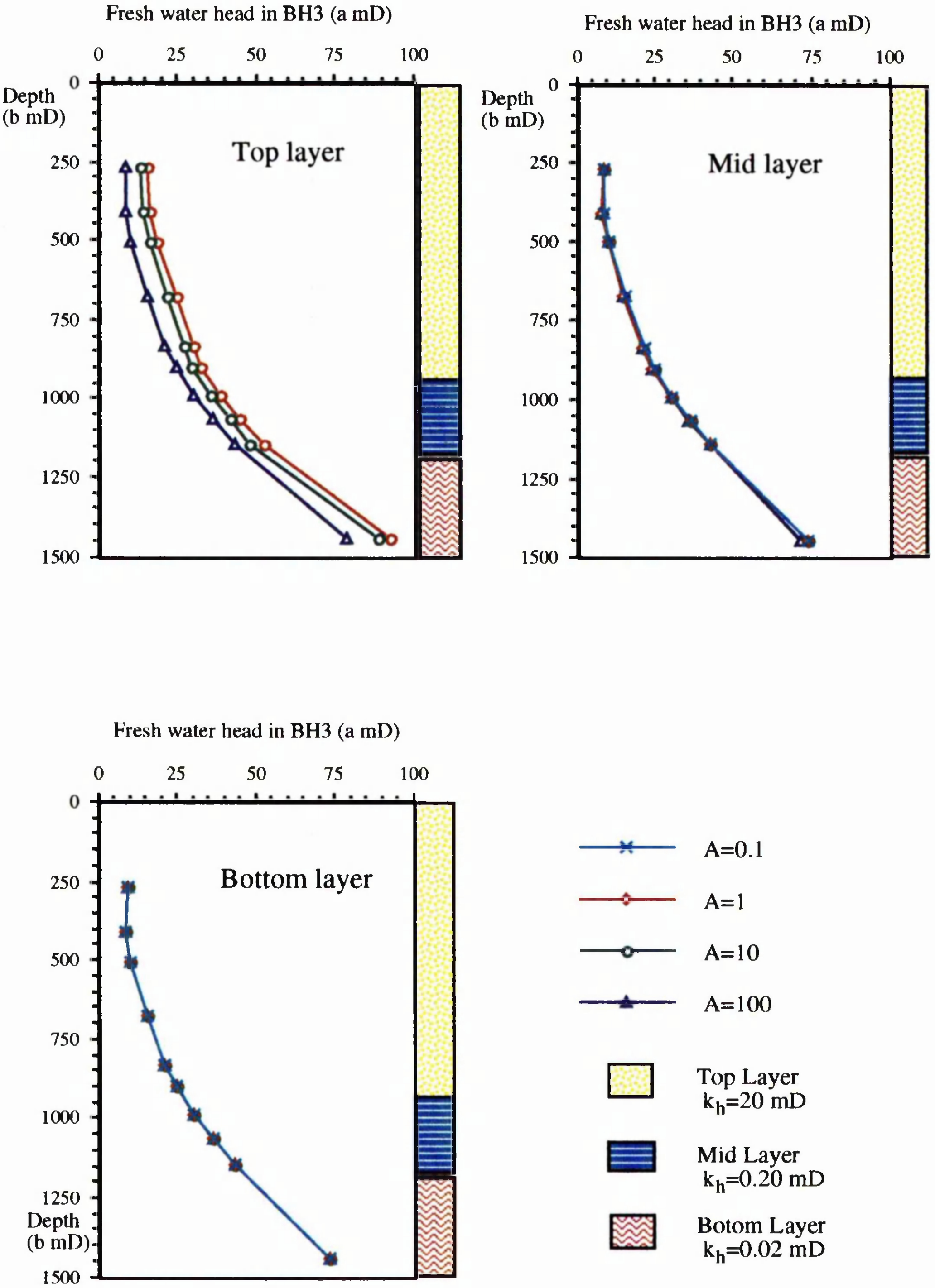


Figure 4-5 Sensitivity test of anisotropy ($A = k_h/k_v$) in the Three-layer Model

The modelled head is not sensitive to the ratio A of horizontal conductivity to vertical conductivity except the top layer.

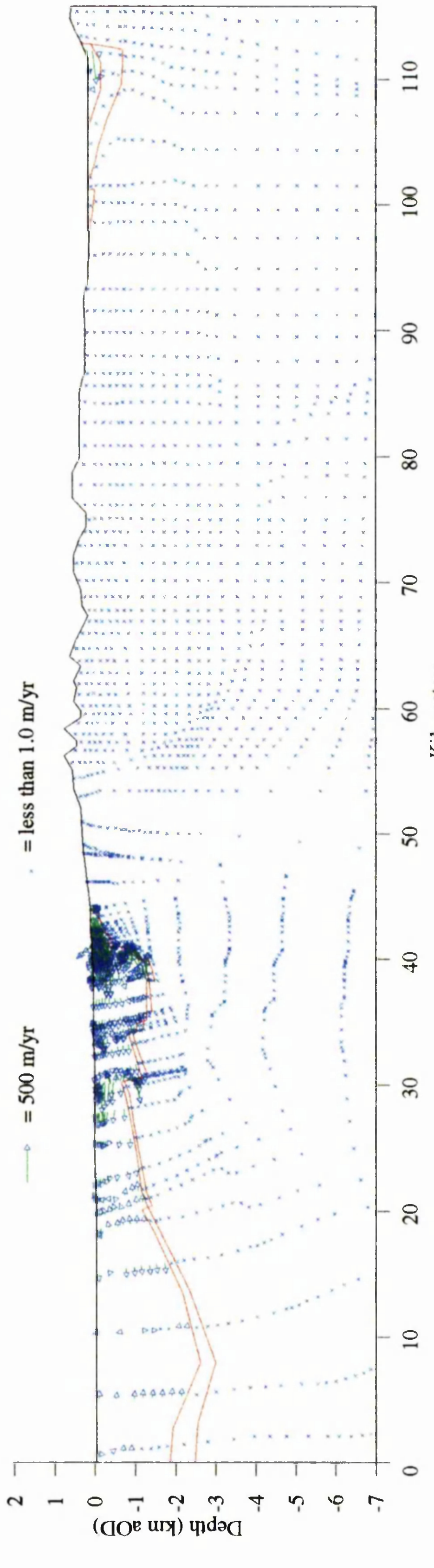


Figure 4-6 Groundwater Velocity from the Three-layer Model

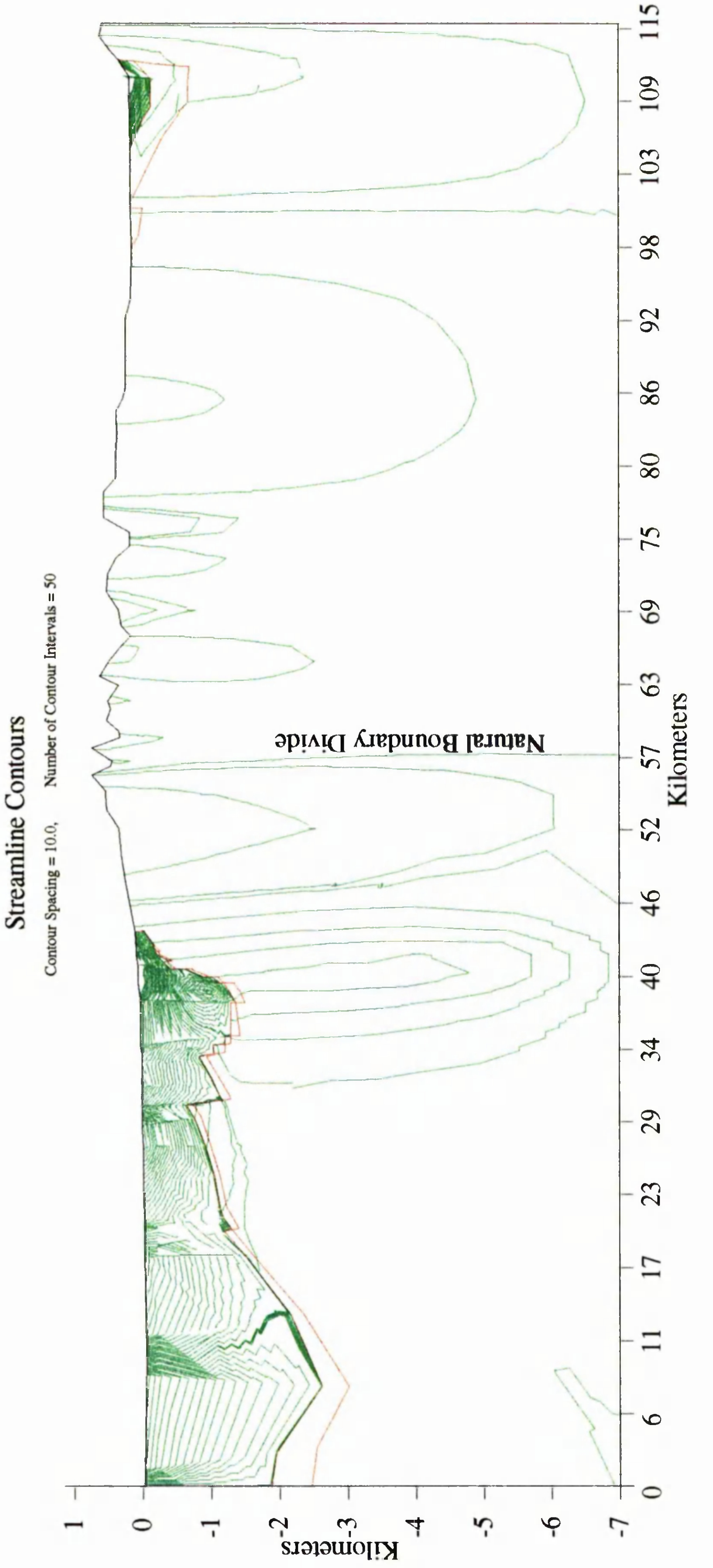


Figure 4-7 Streamlines from the Three-layer Model

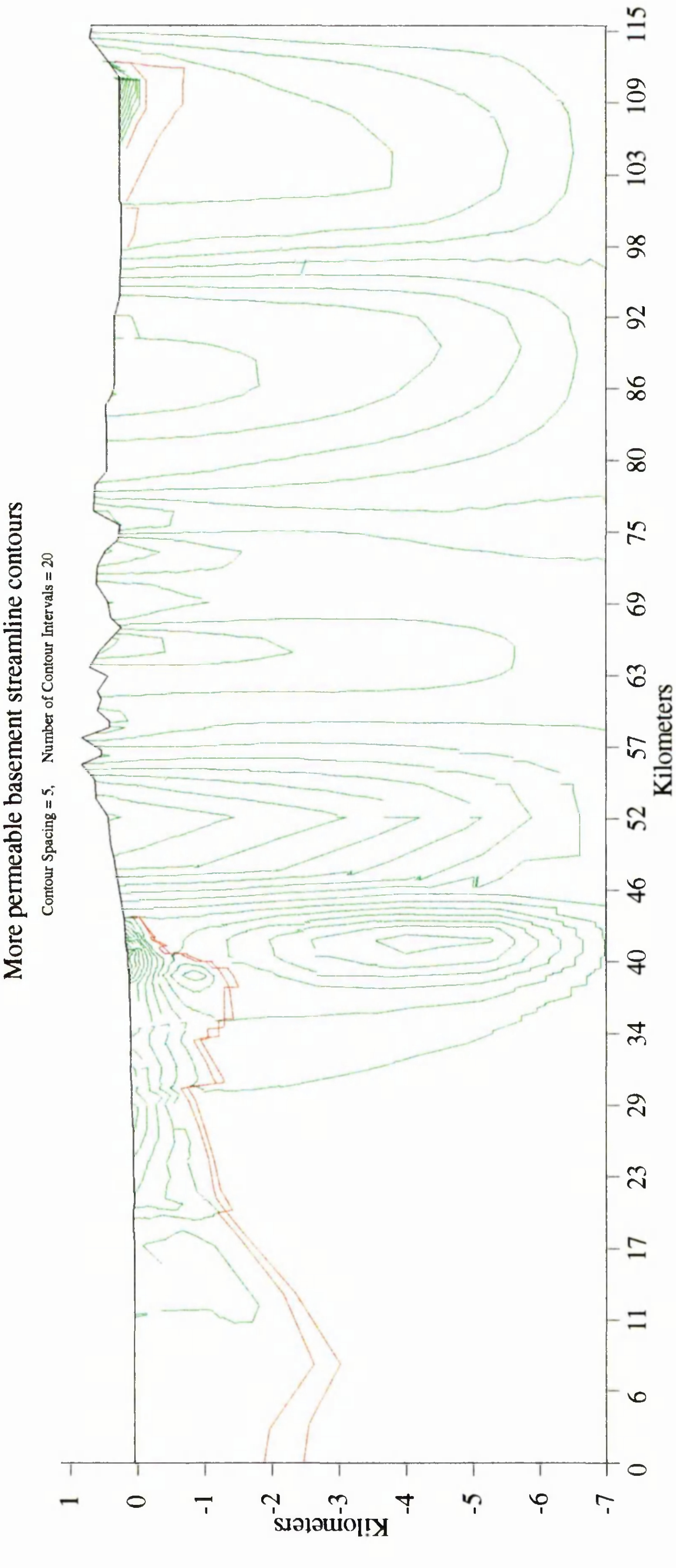


Figure 4-8 Streamlines from the Three-layer Model (More permeable basement)

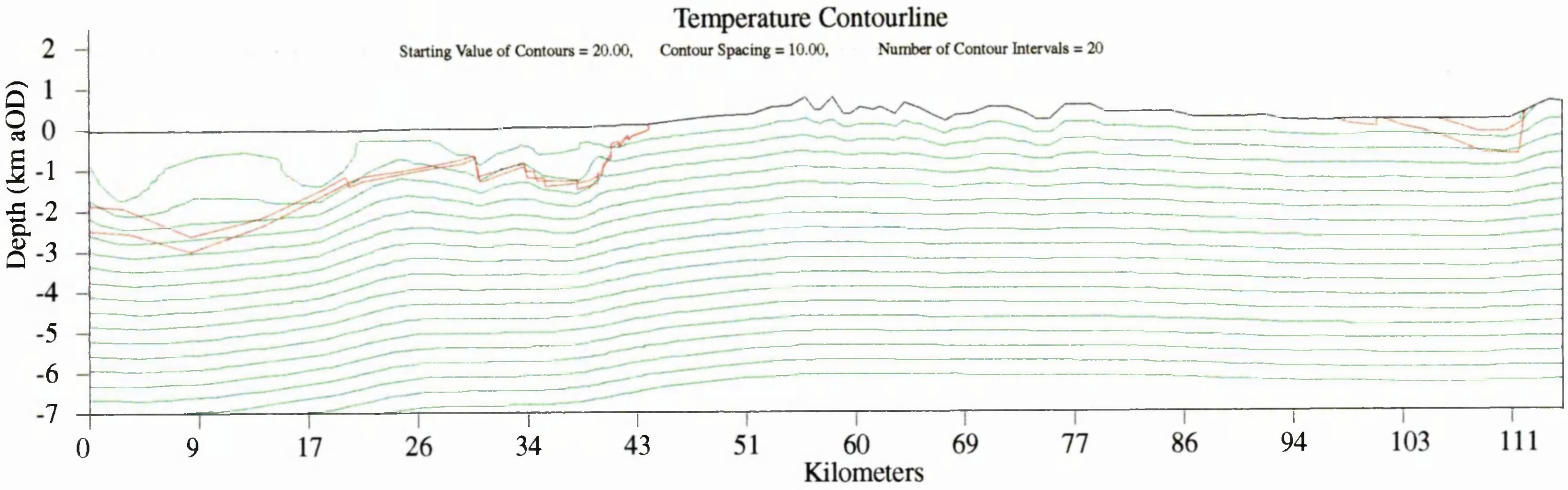


Figure 4-9 Temperature distribution from the Three-layer Model

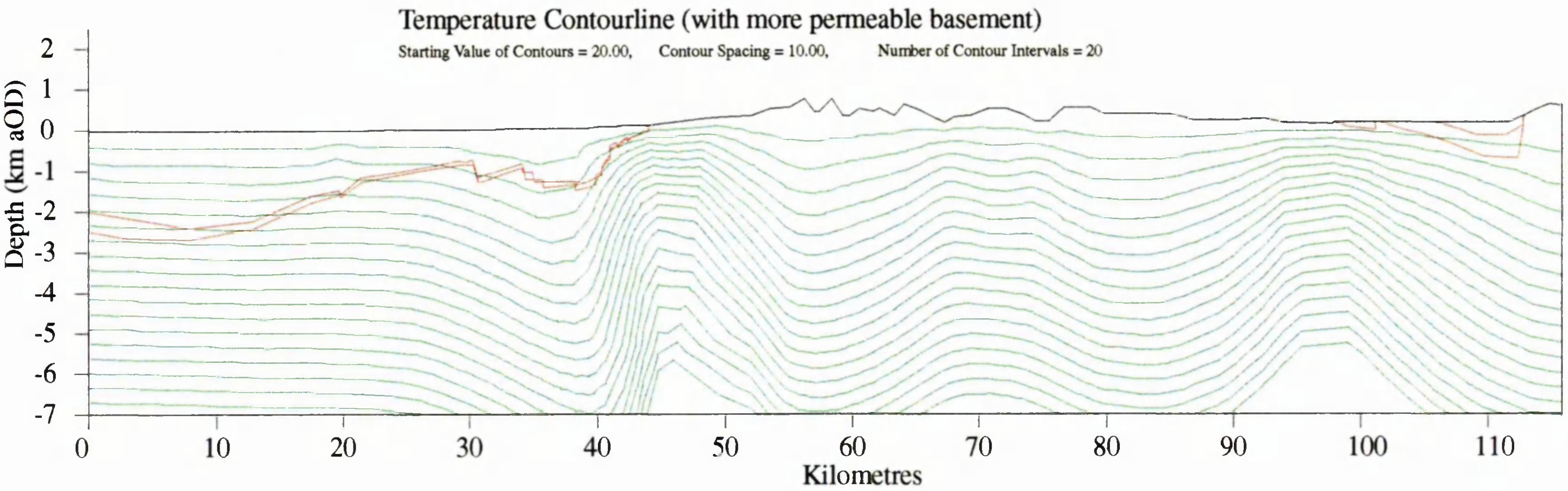


Figure 4-10 Temperature distribution (more permeable basement) from the Three-layer Model

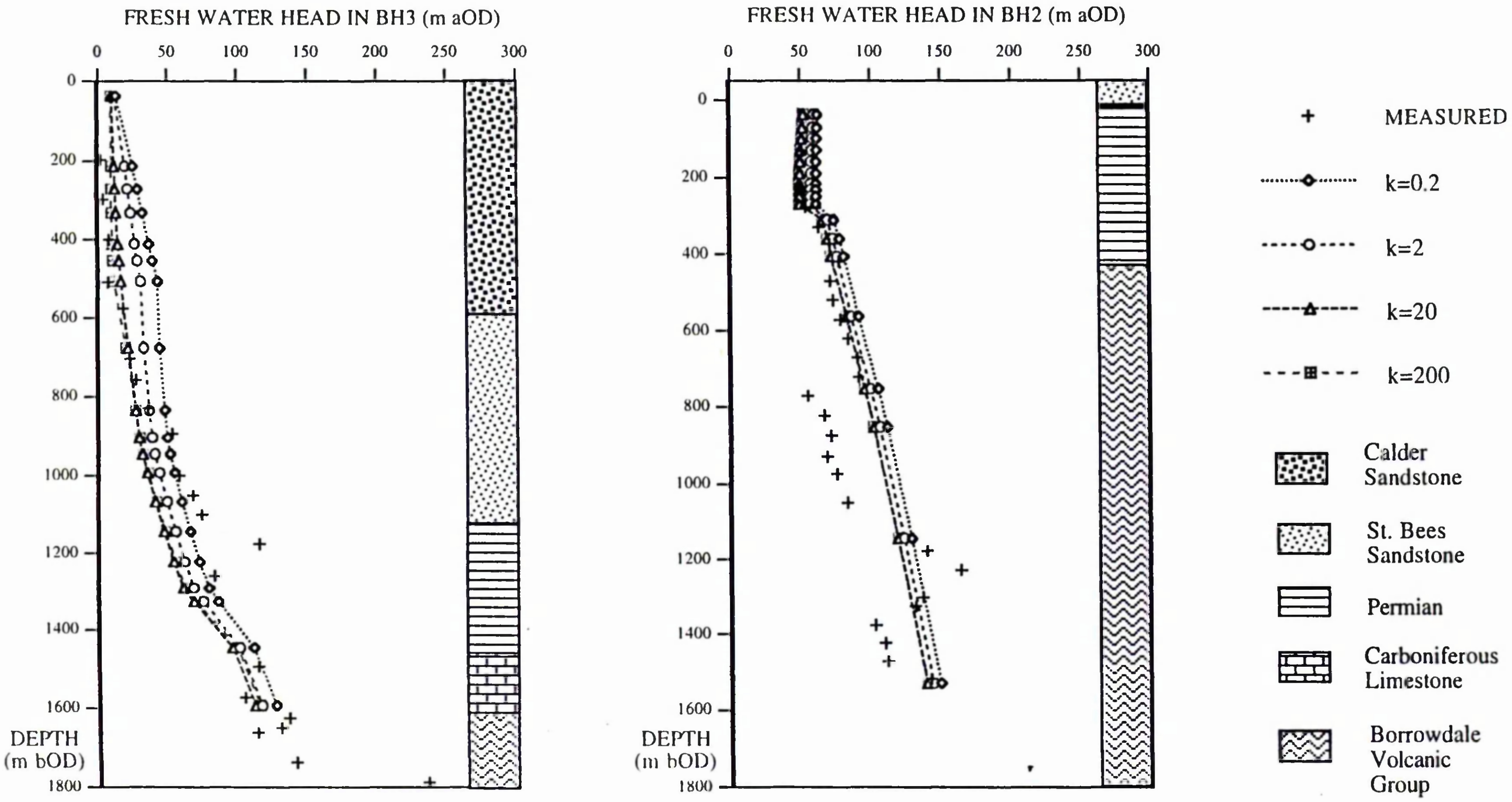


Figure 4-11 Permeability test of Calder Sandstone in the Seven-layer Model

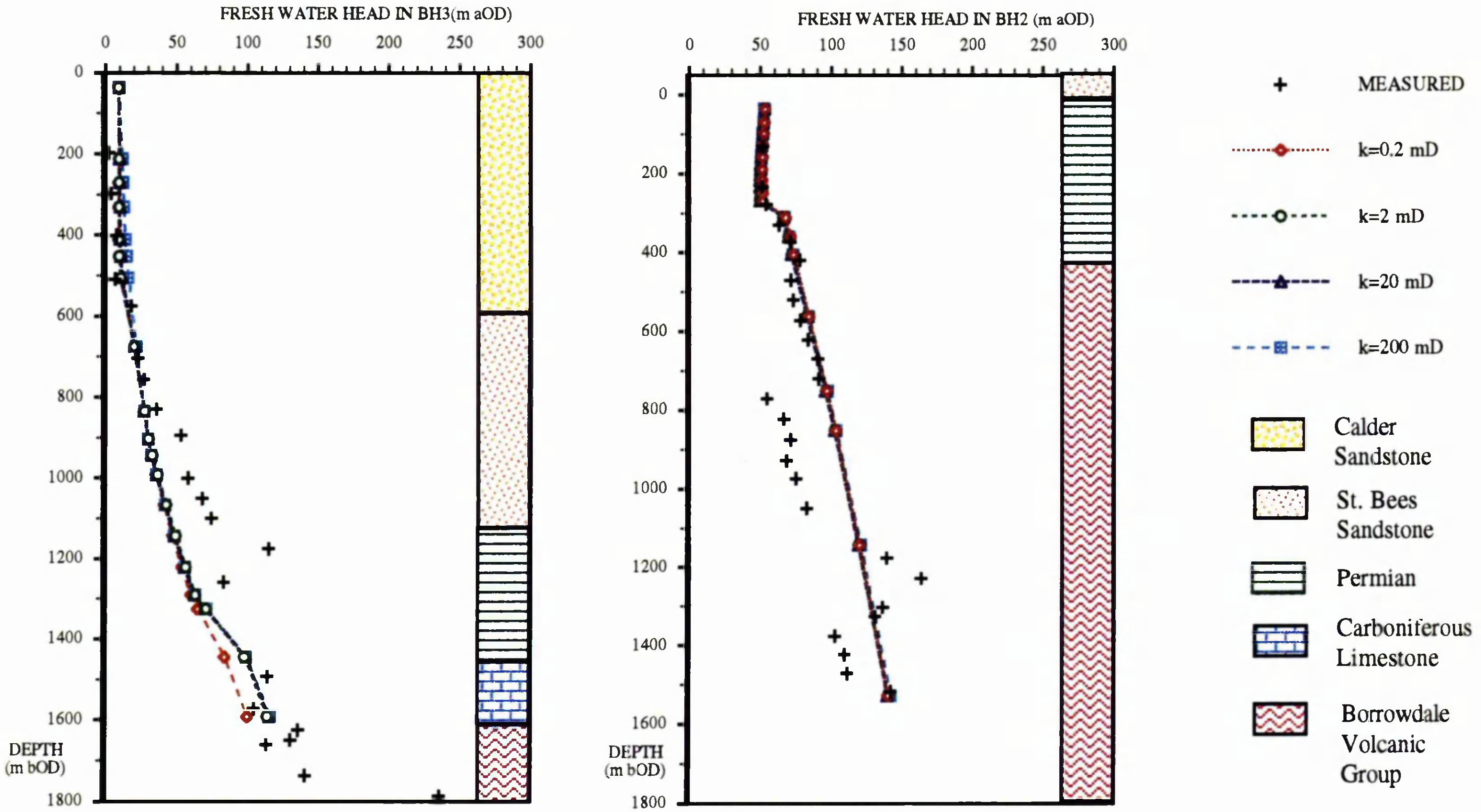


Figure 4-12 Sensitivity Test of Permeability on St Bees Sandstone in the Seven-layer Model
The permeability was tested from 0.2 mD to 200 mD, and the modelled head is not sensitive to the change.

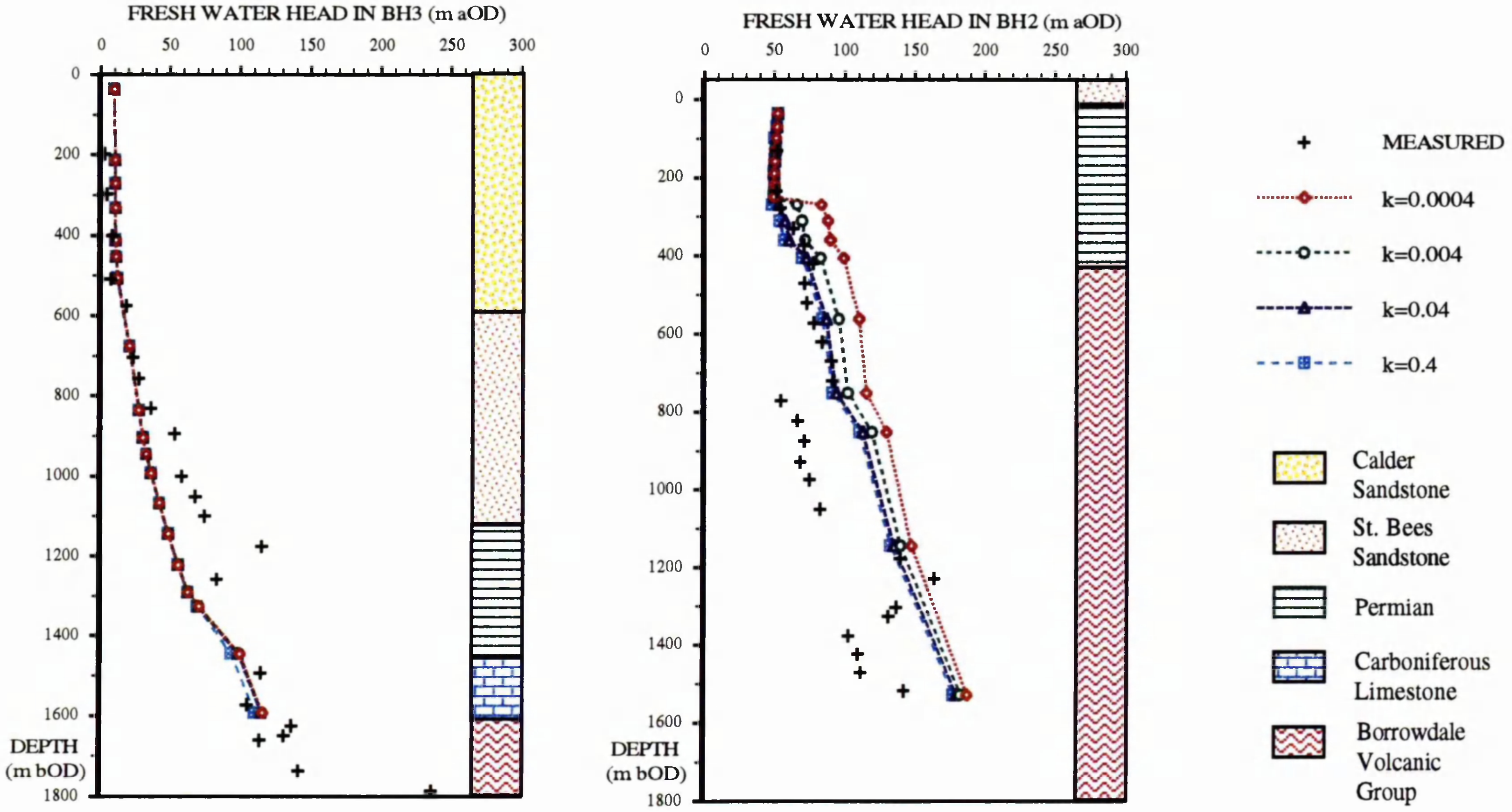


Figure 4-13 Sensitivity Test of Permeability on the Permian in the Seven-layer Model
The modelled head responds too high in BH2 when the permeability of the Premian is too small

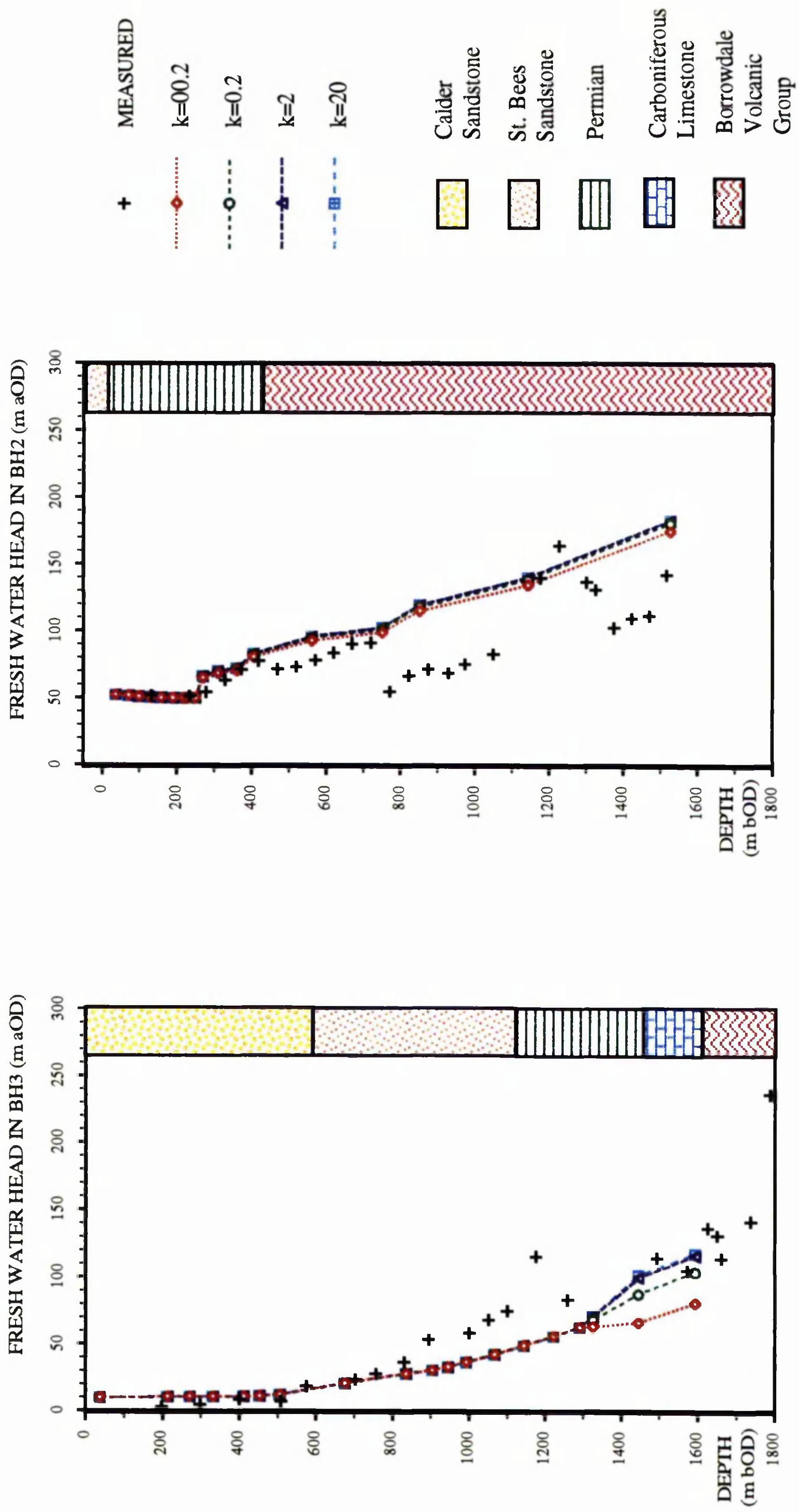


Figure 4-14 Sensitivity Test of Permeability on the Carboniferous Limestone in the Seven-layer Model

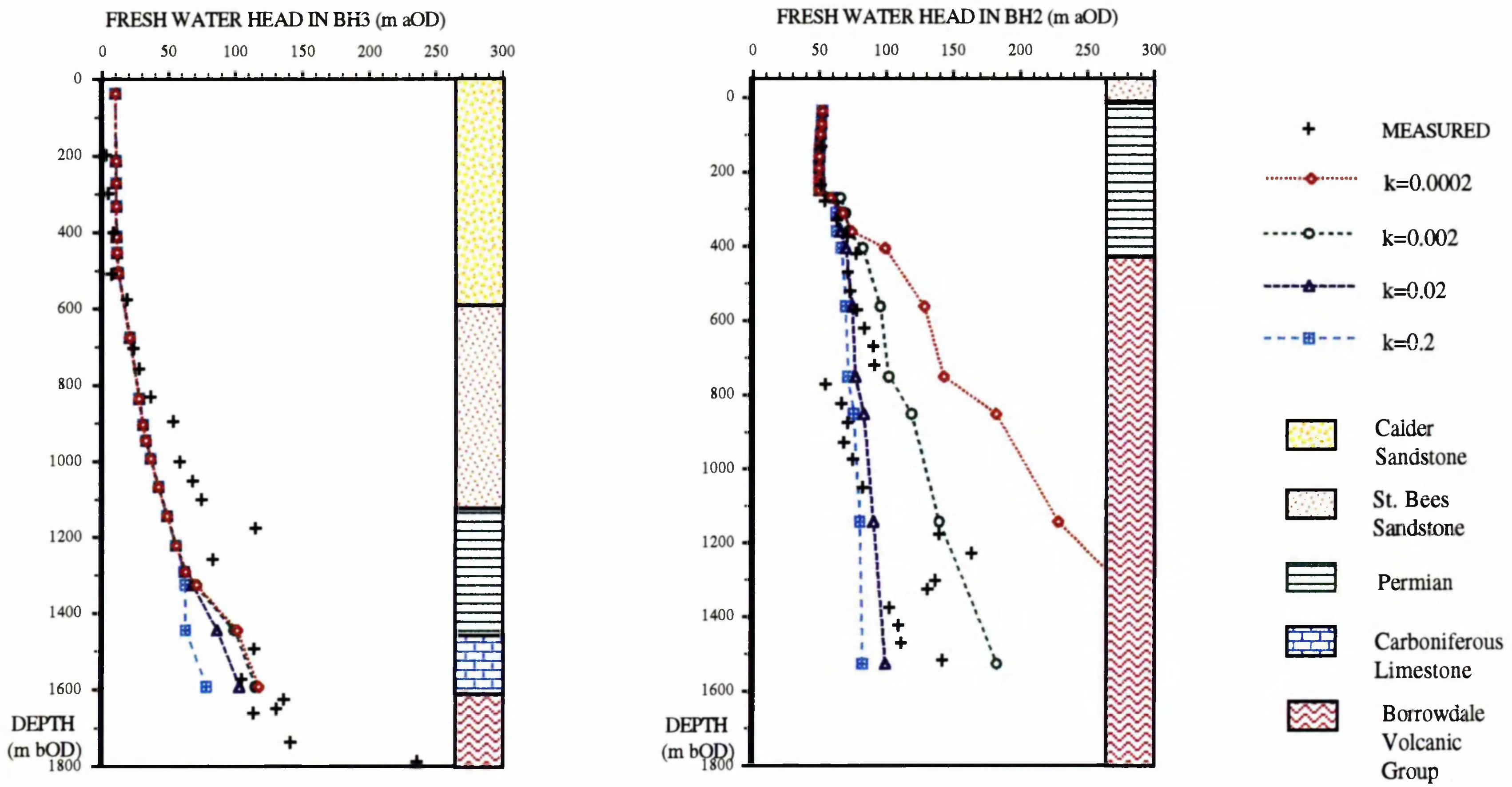
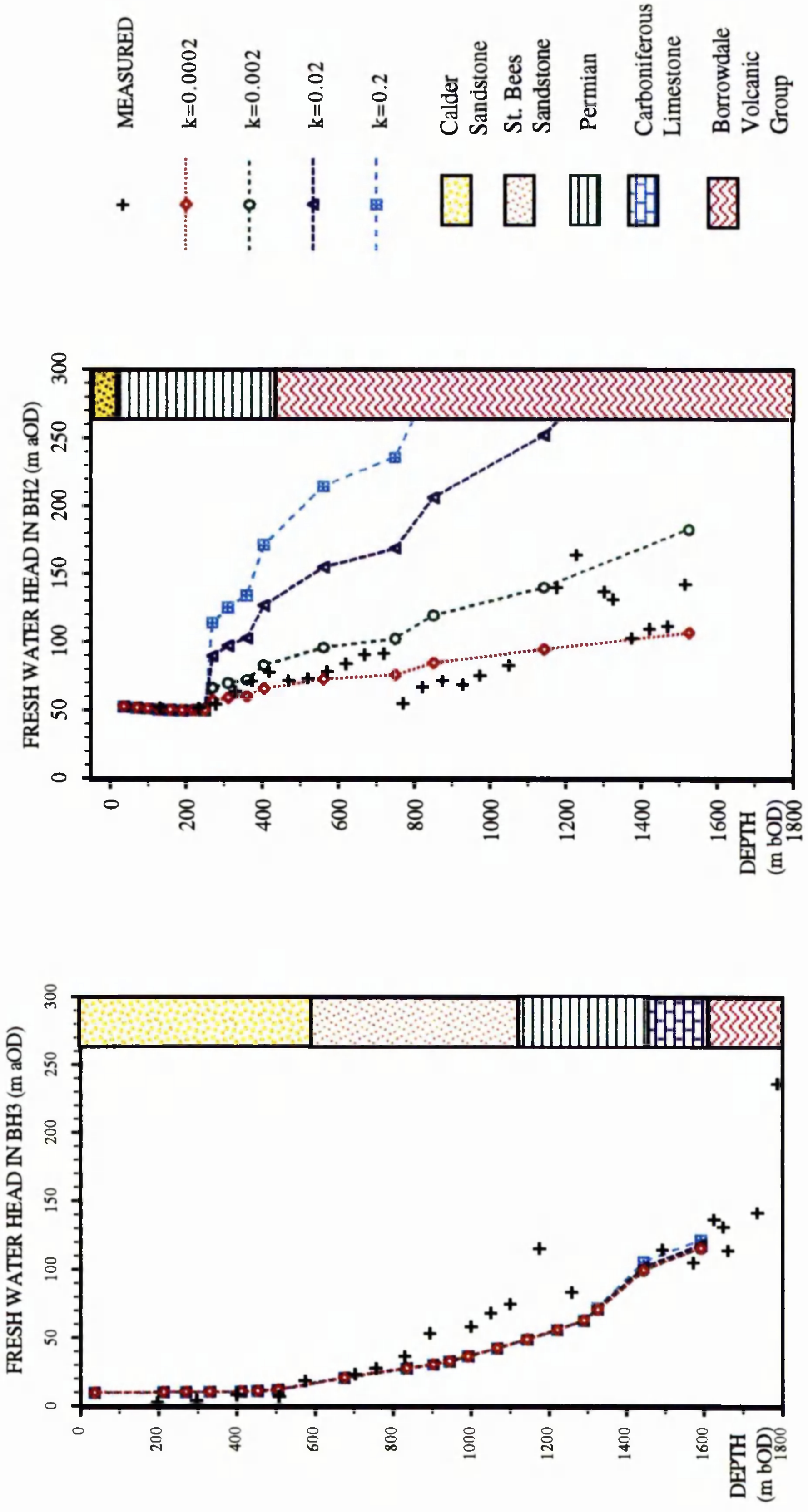


Figure 4-15 Permeability Test of Borrowdale Volcanic Group in Seven-layer Model
The modelled head is very sensitive to the permeability of the BVG, in paricular in BH2, when the permeability is less than 0.002mD, the computed head is far above the measured value



Figutre 4-16 Sensitivity Test of Permeability on the Slate in the Seven-layer Model

The modelled head is also very sensitive to the permeability of the Slate, the higher permeability, the higher predicted head.

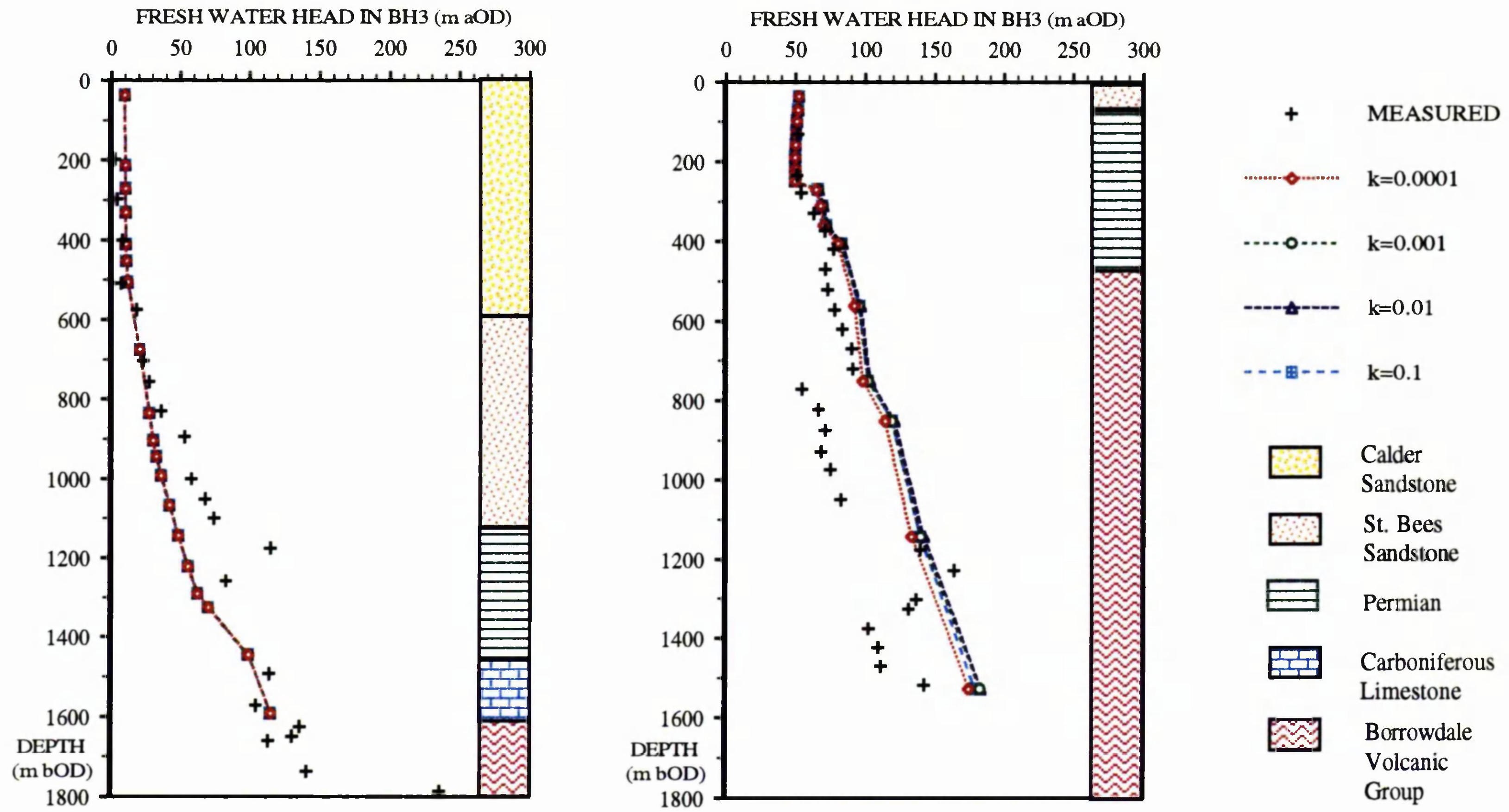


Figure 4-17 Sensitivity Test of Permeability on the Granite in the Seven-layer Model
The modelled head is not sensitive to the permeability of the Granite

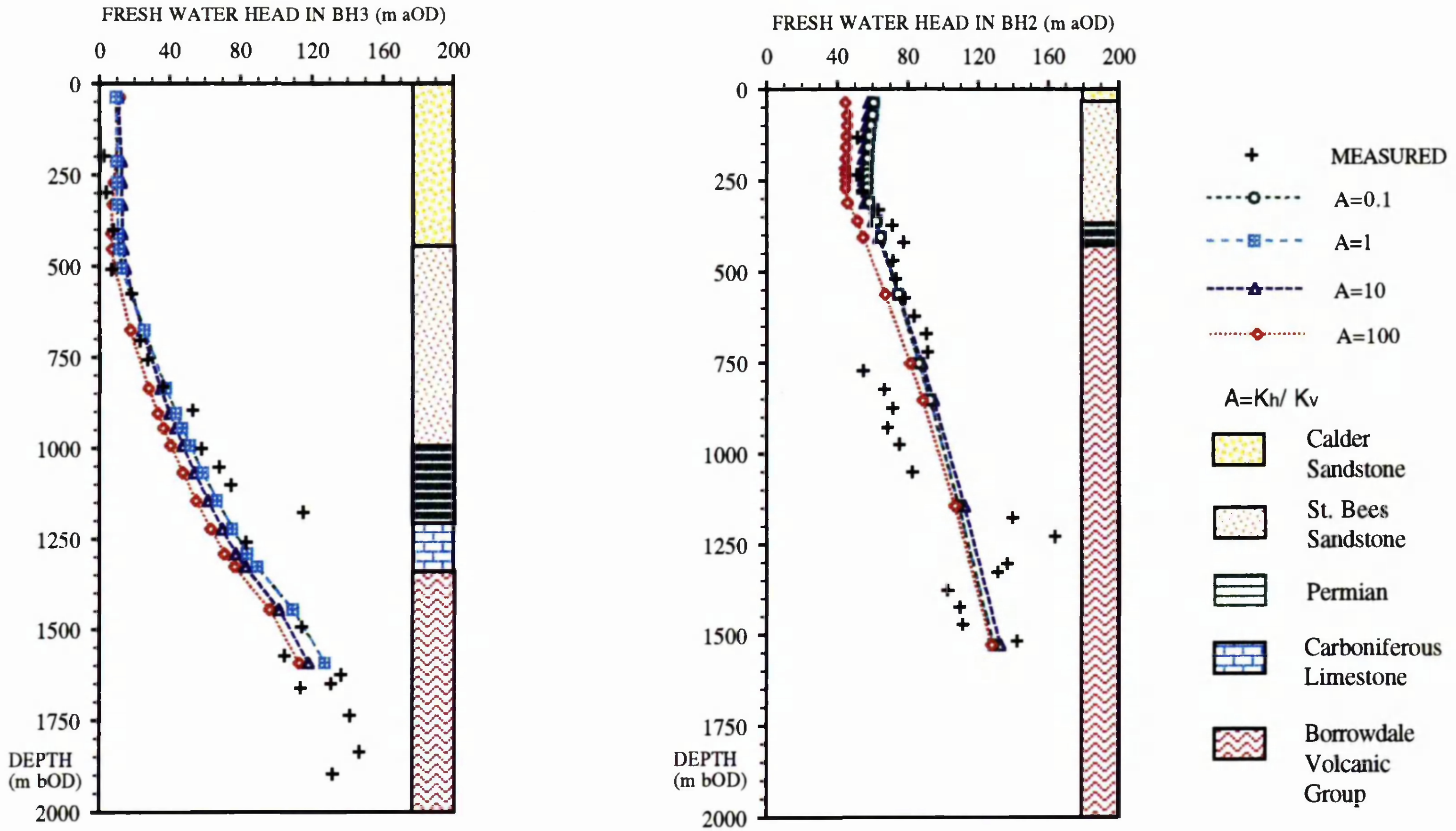


Figure 4-18 Sensitivity test of anisotropy in the Calder Sandstone in the Seven Layer Model
The anisotropy is represented by the ratio of horizontal hydraulic conductivity to vertical hydraulic conductivity, A=Kh/Kv

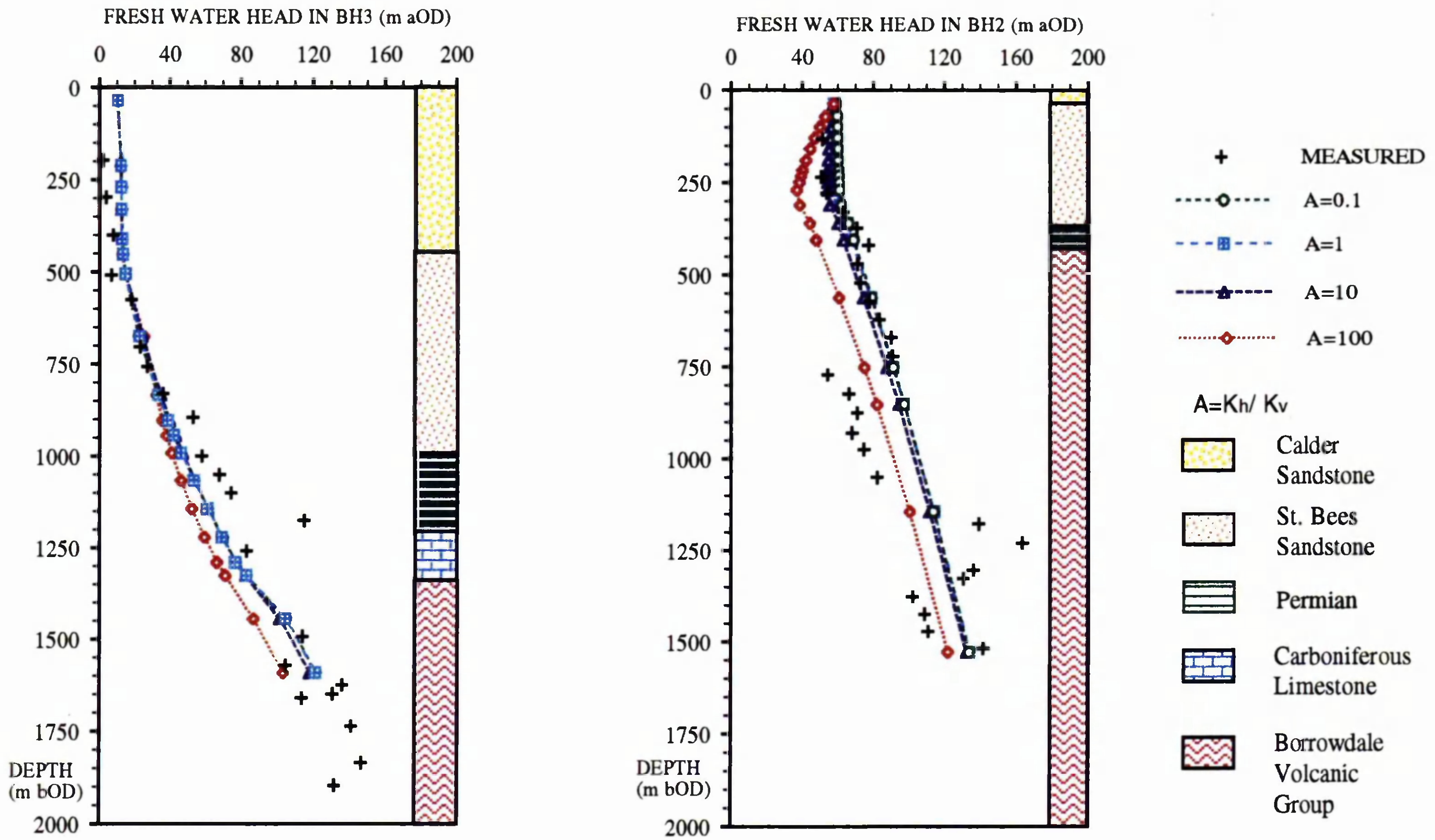


Figure 4-19 Sensitivity test of anisotropy in the St Bees Sandstone in the Seven-layer Model

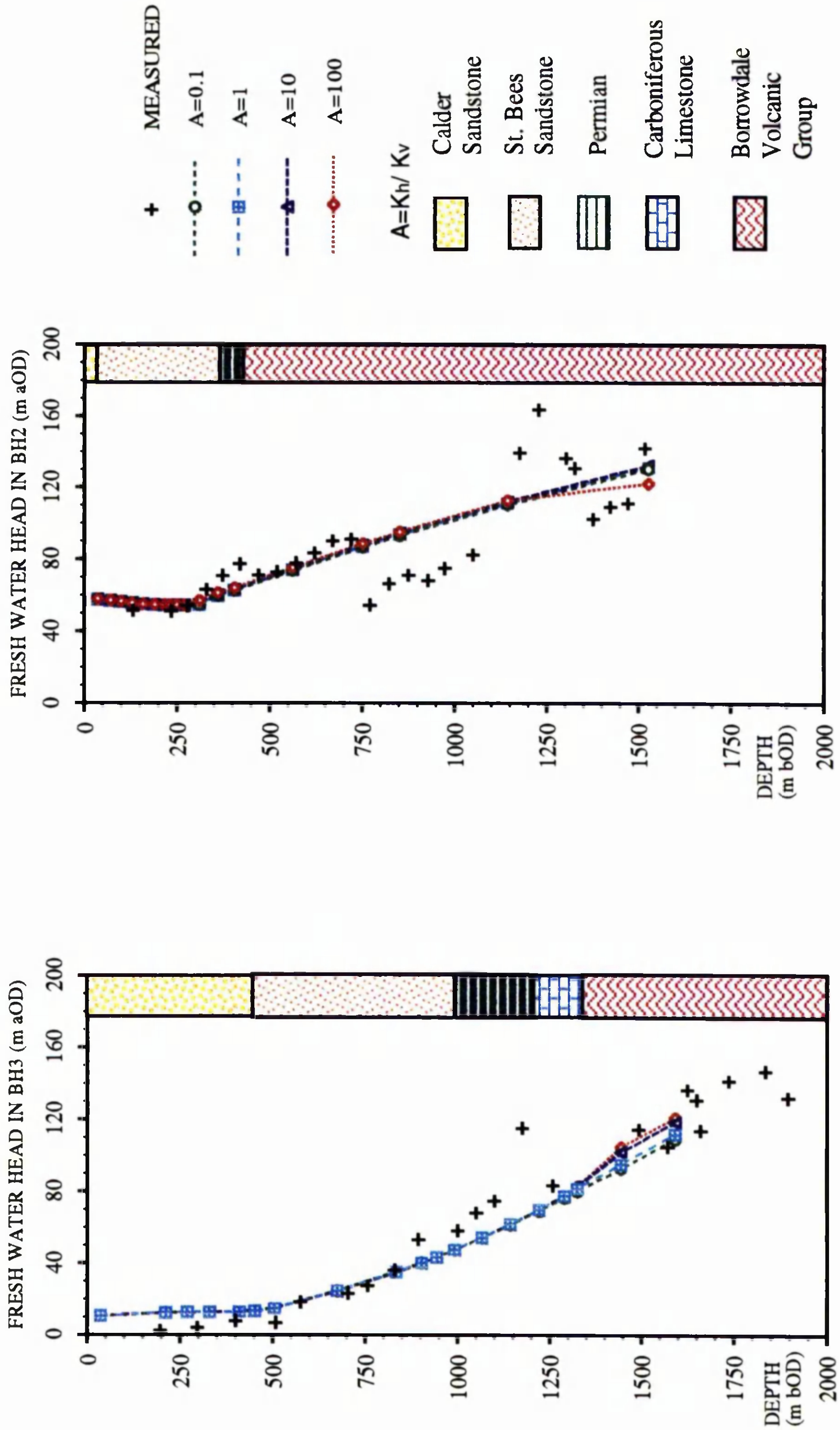


Figure 4-20 Sensitivity test of anisotropy in the Permian in the Seven-layer Model

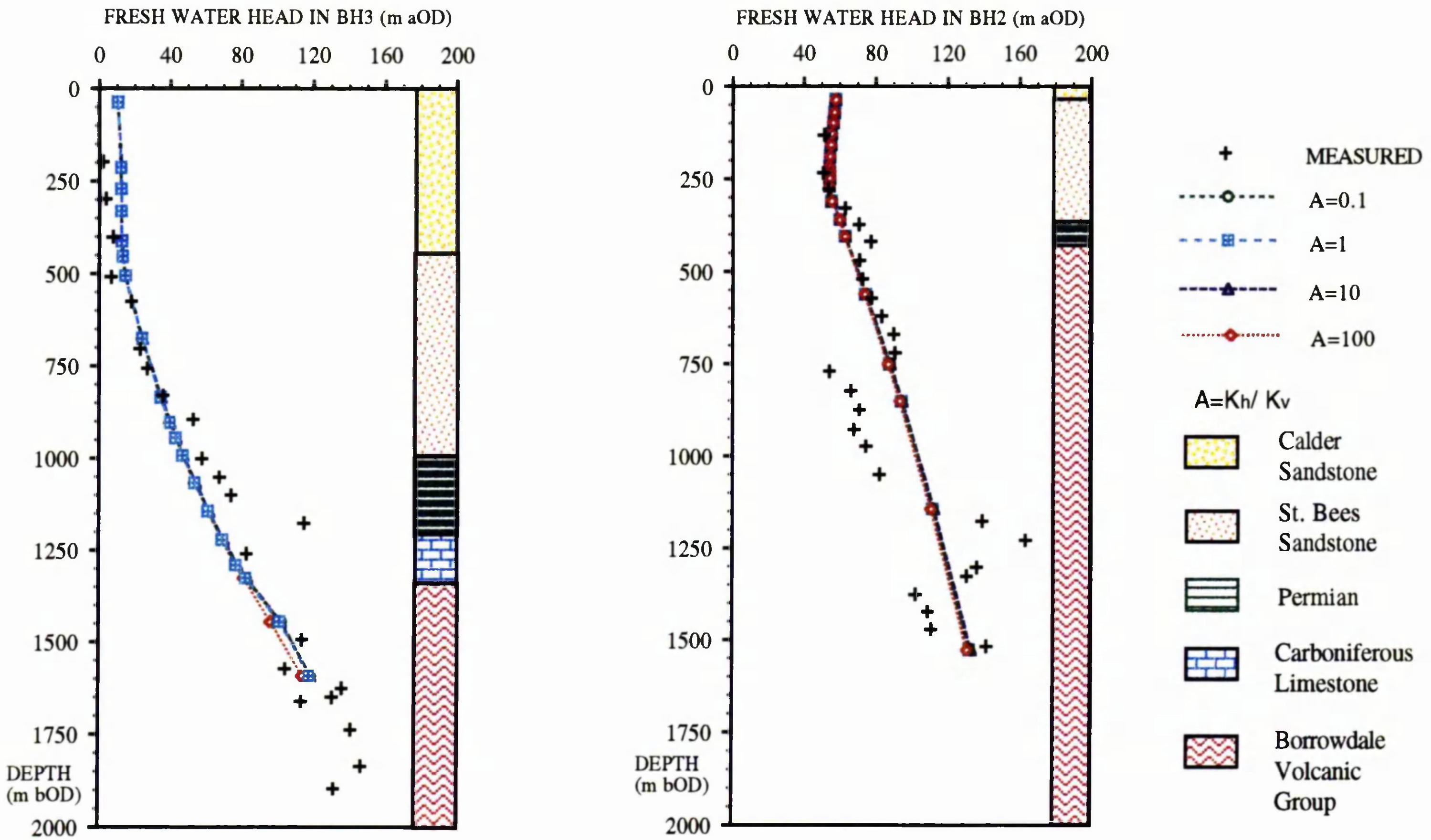


Figure 4-21 Sensitivity test of anisotropy in the Carboniferous Limestone in the Seven-layer Model

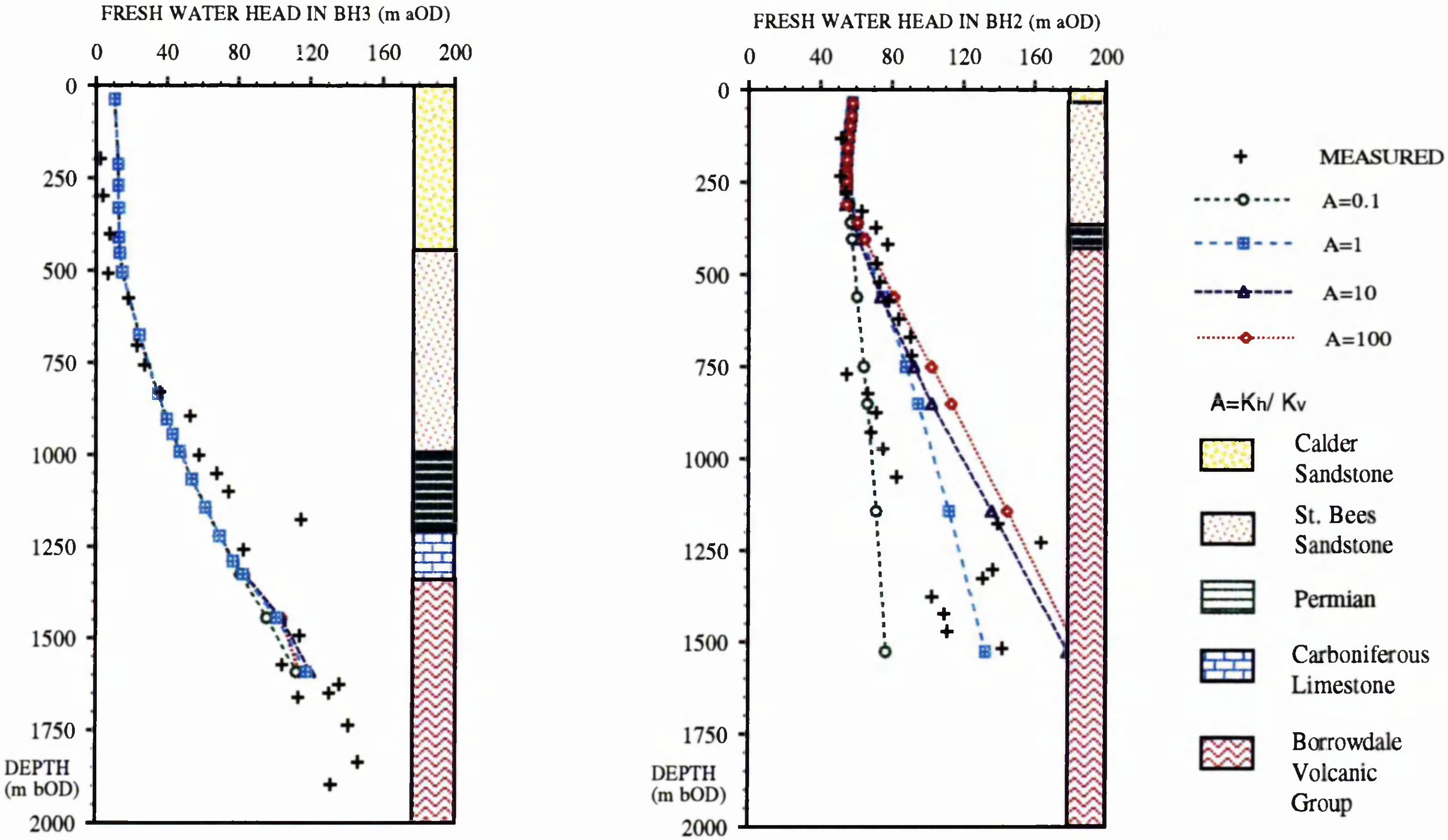


Figure 4-22 Sensitivity test of anisotropy in the Borrowdale Volcanic Group in the Seven Layer Model
The modelled head is very sensitive to the anisotropy of the BVG

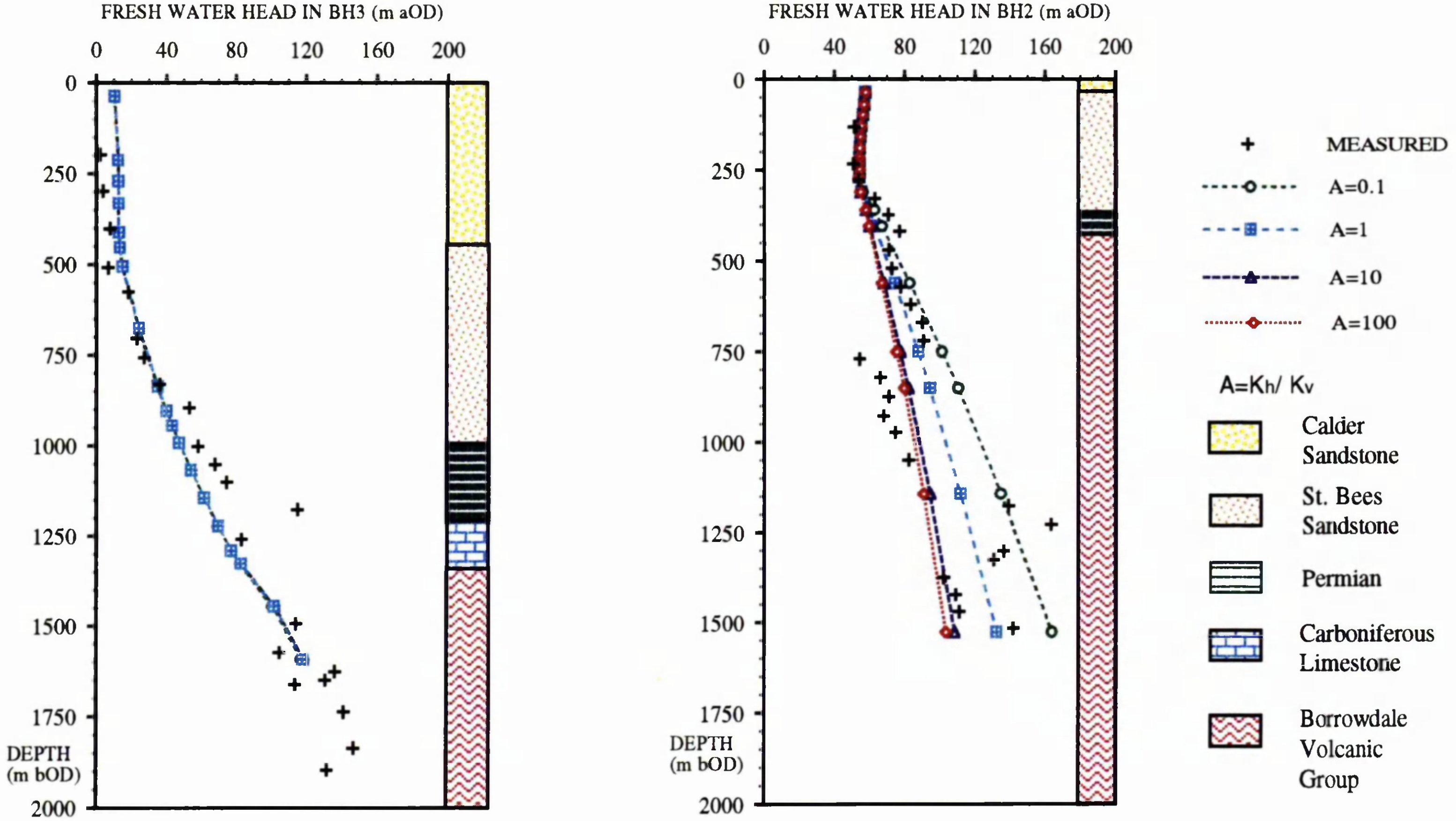


Figure 4-23 Sensitivity test of anisotropy in the Skiddaw Group in the Seven-layer Model
The modelled head in BH2 is also sensitive to the anisotropy of the Skiddaw Group

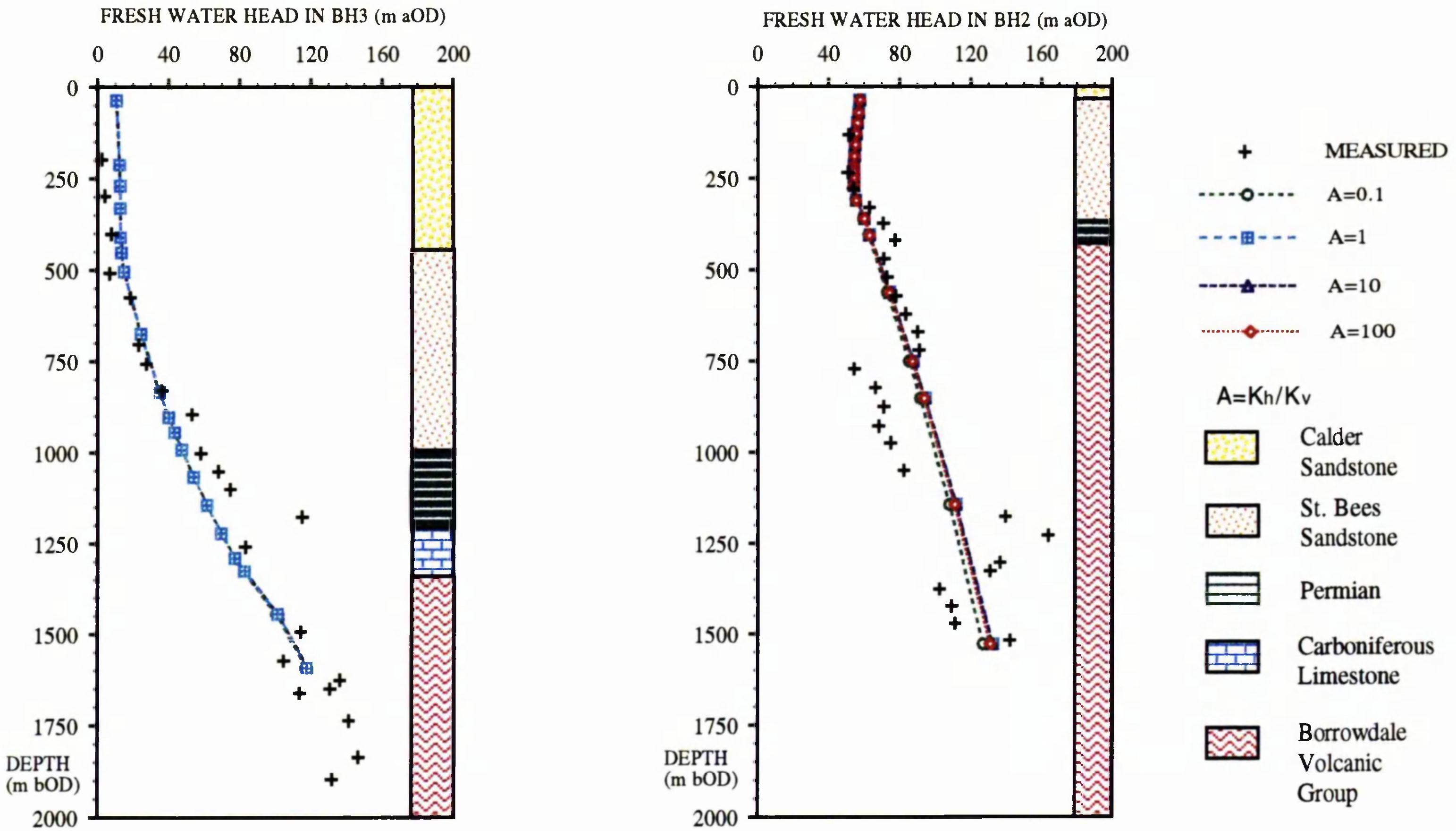


Figure 4-24 Sensitivity test of anisotropy in the Granite in the Seven-layer Model
The modelled head is not sensitive to the anisotropy of the Granite

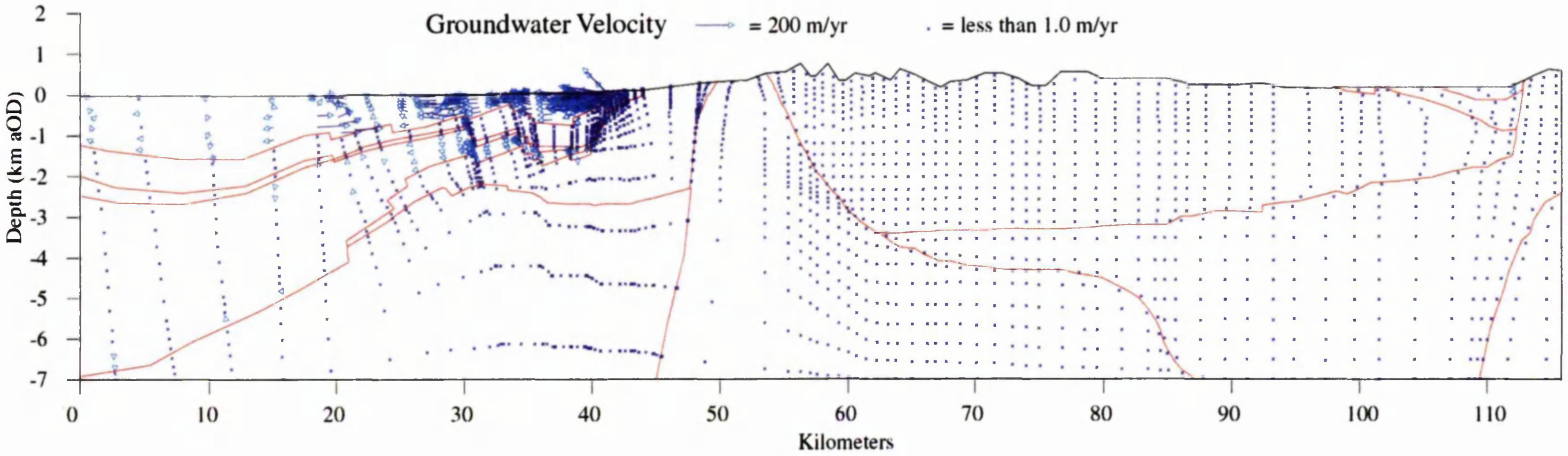


Figure 4-25 Groundwater Velocity from the Seven-layer Model

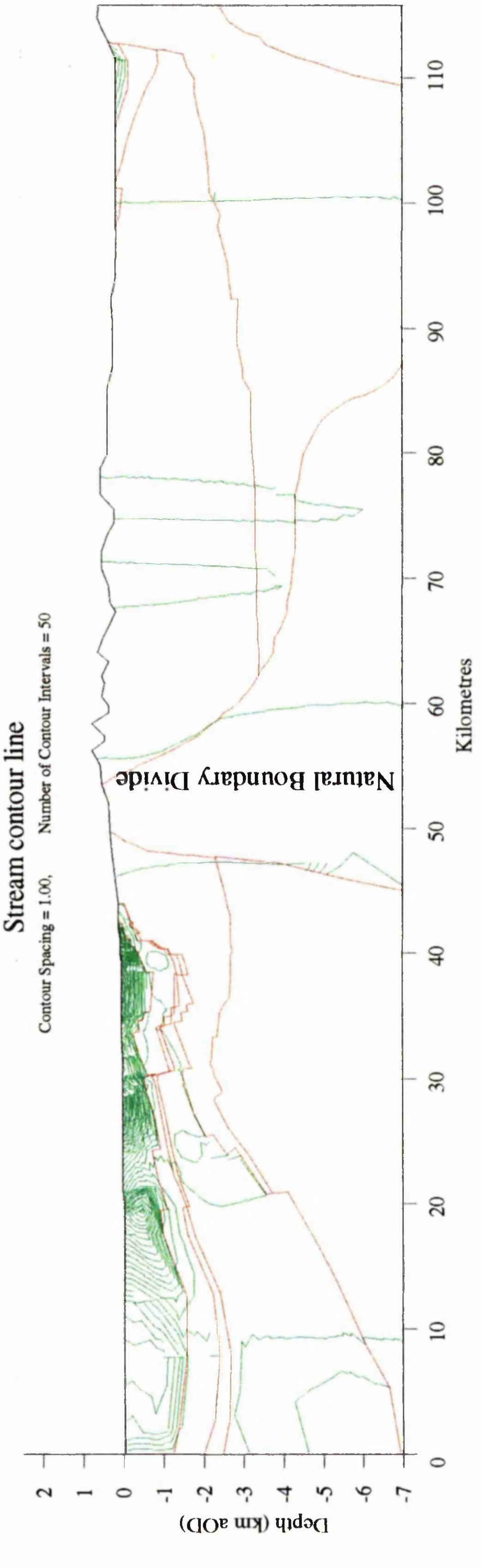


Figure 4-26 Stream lines from the Seven-layer Model

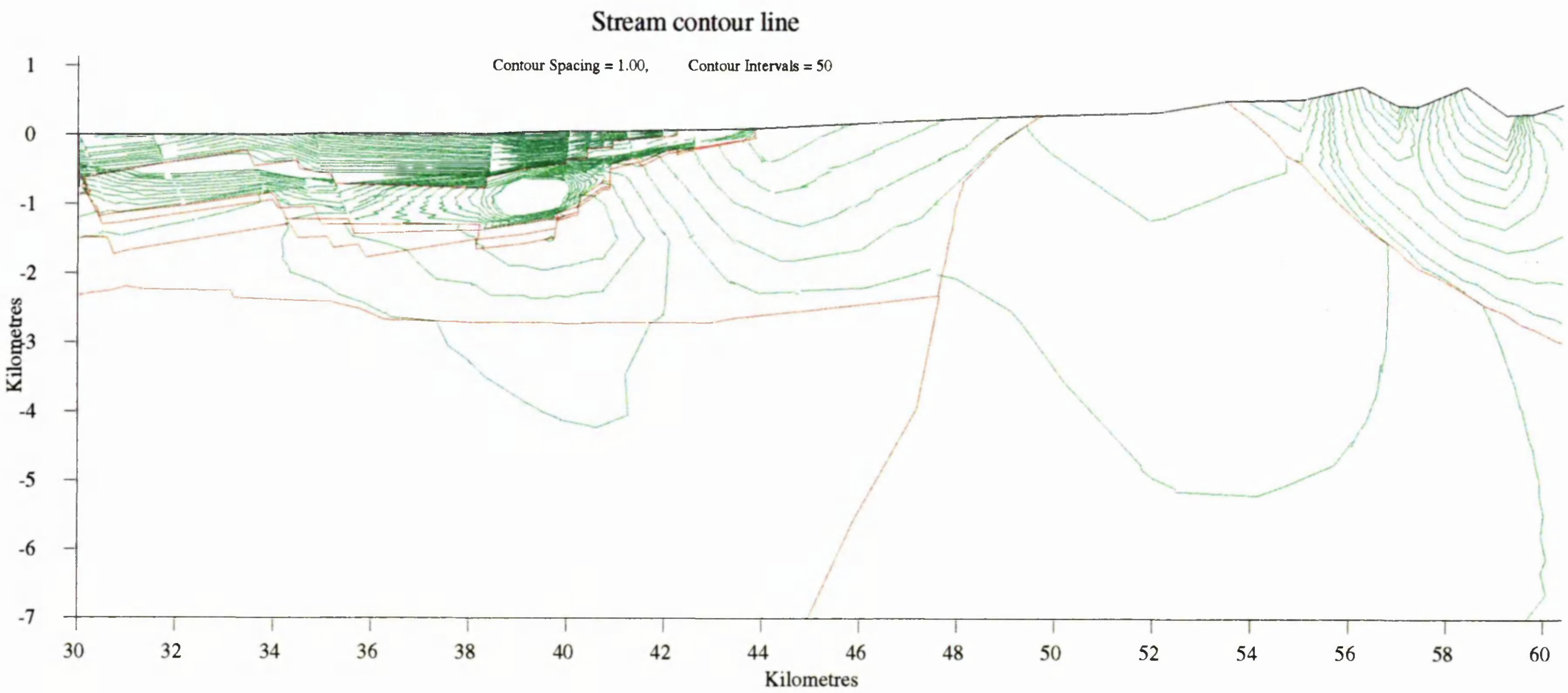


Figure 4-27 Stream lines at Sellafield from the Seven-layer Model

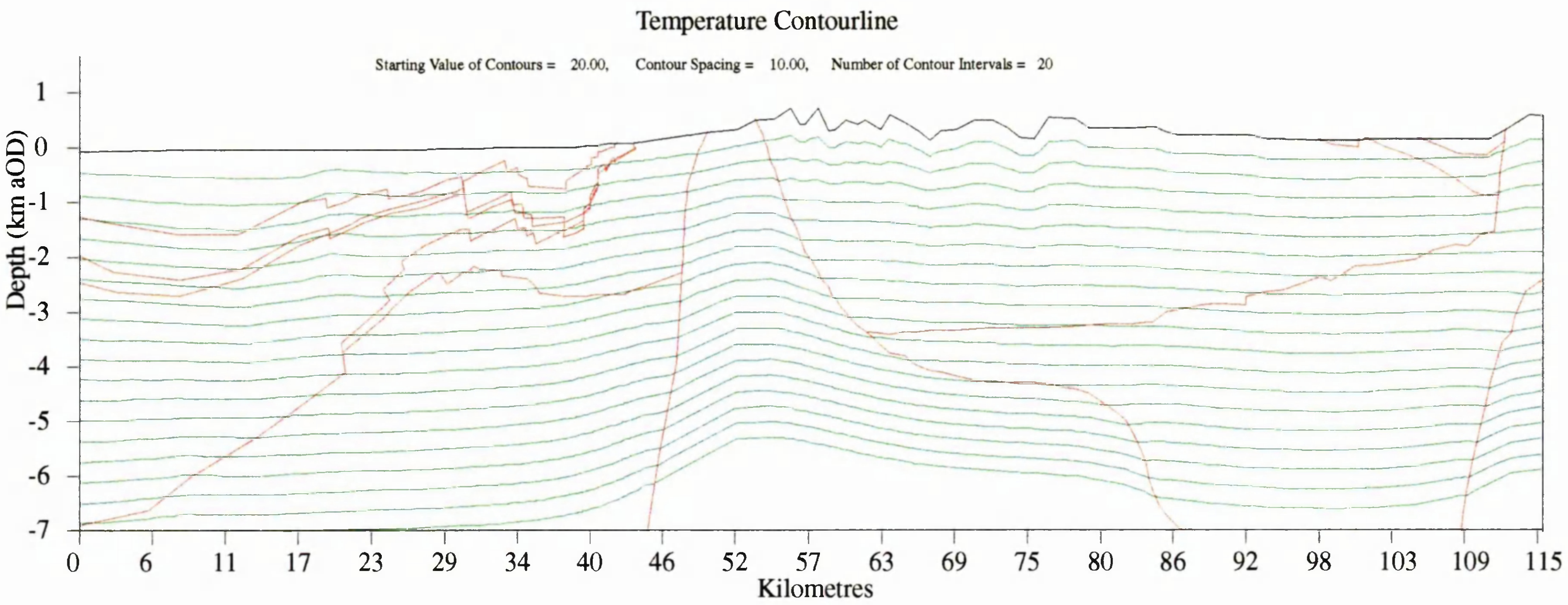


Figure 4-28 Temperature distribution from the Seven-Layer Model

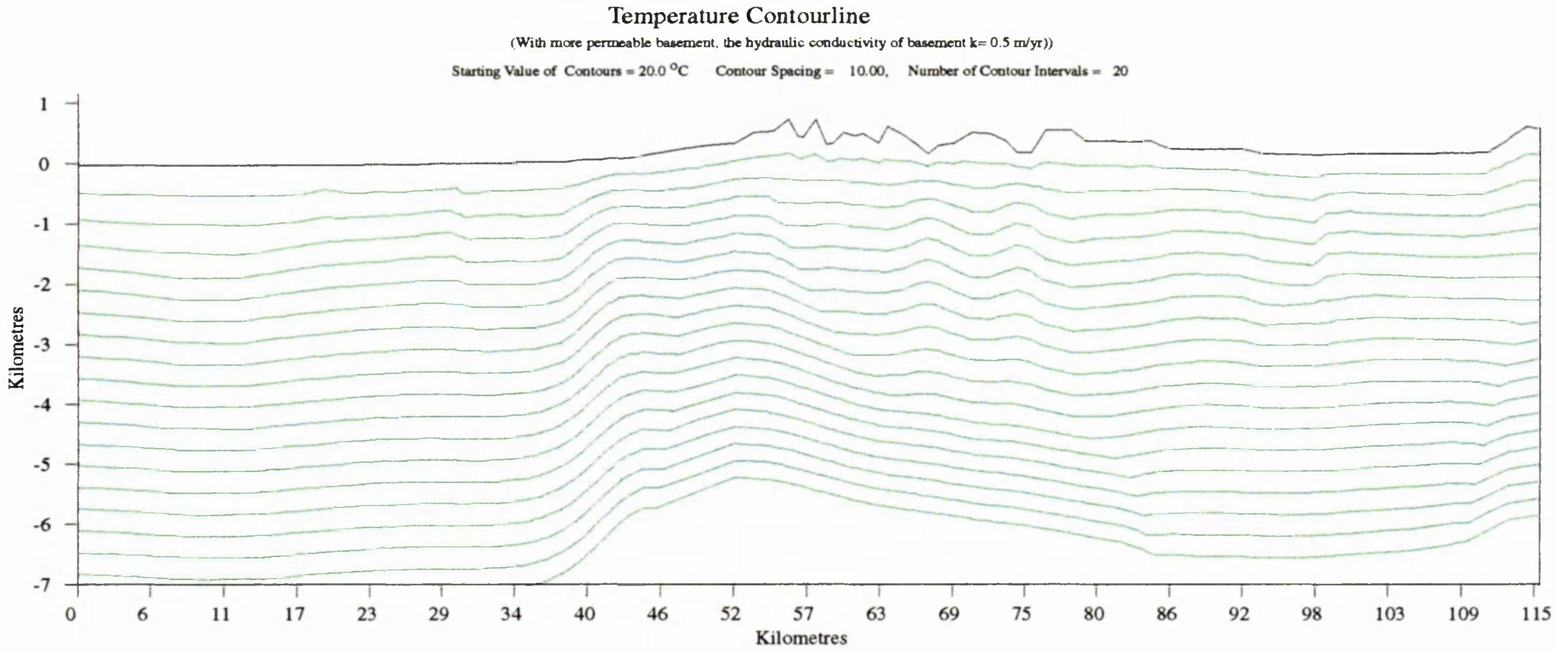


Figure 4-29 Temperature distribution (more permeable basement) from the Seven-layer Model

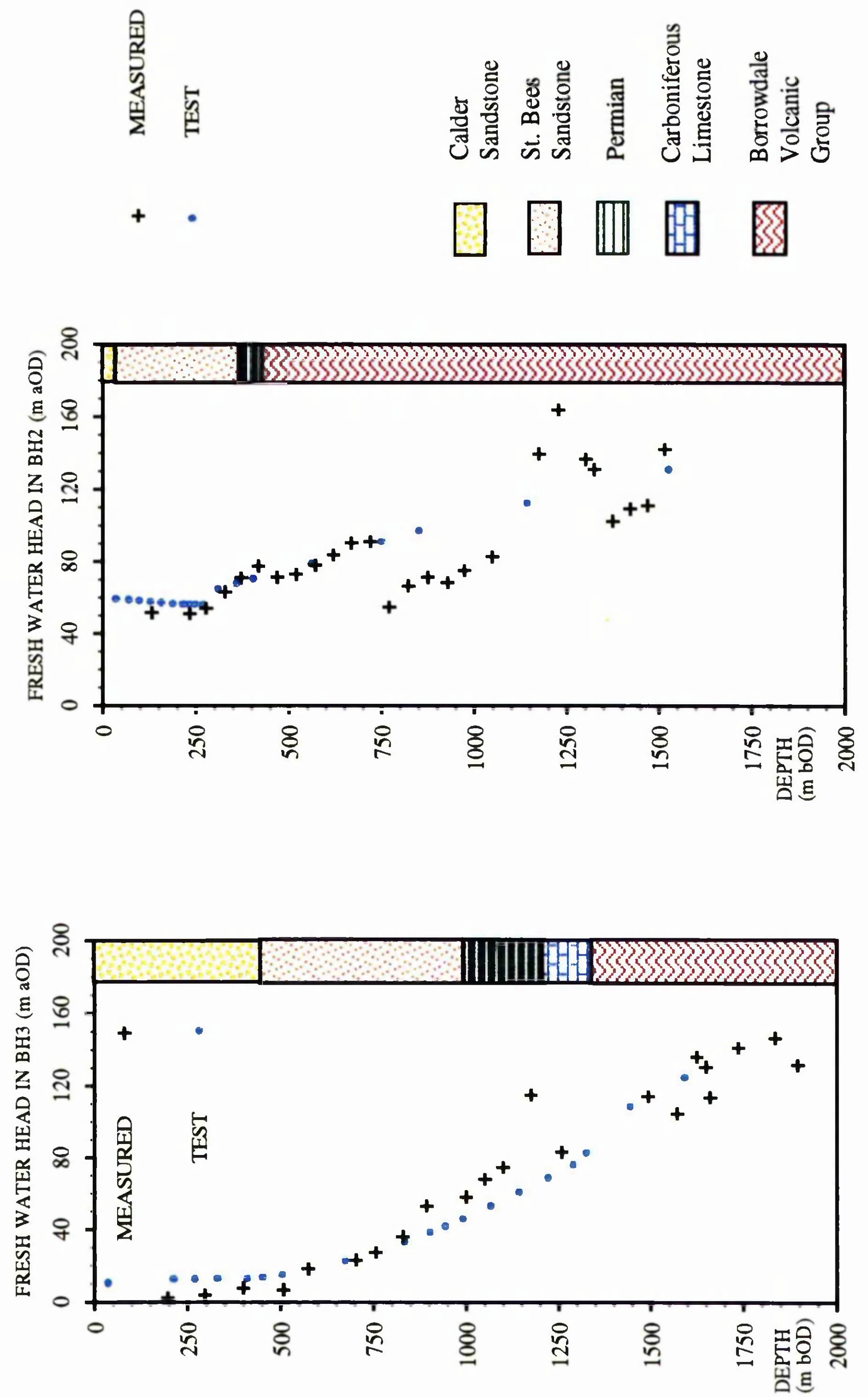


Figure 4-30 The best fit result from the Seven-layer Model

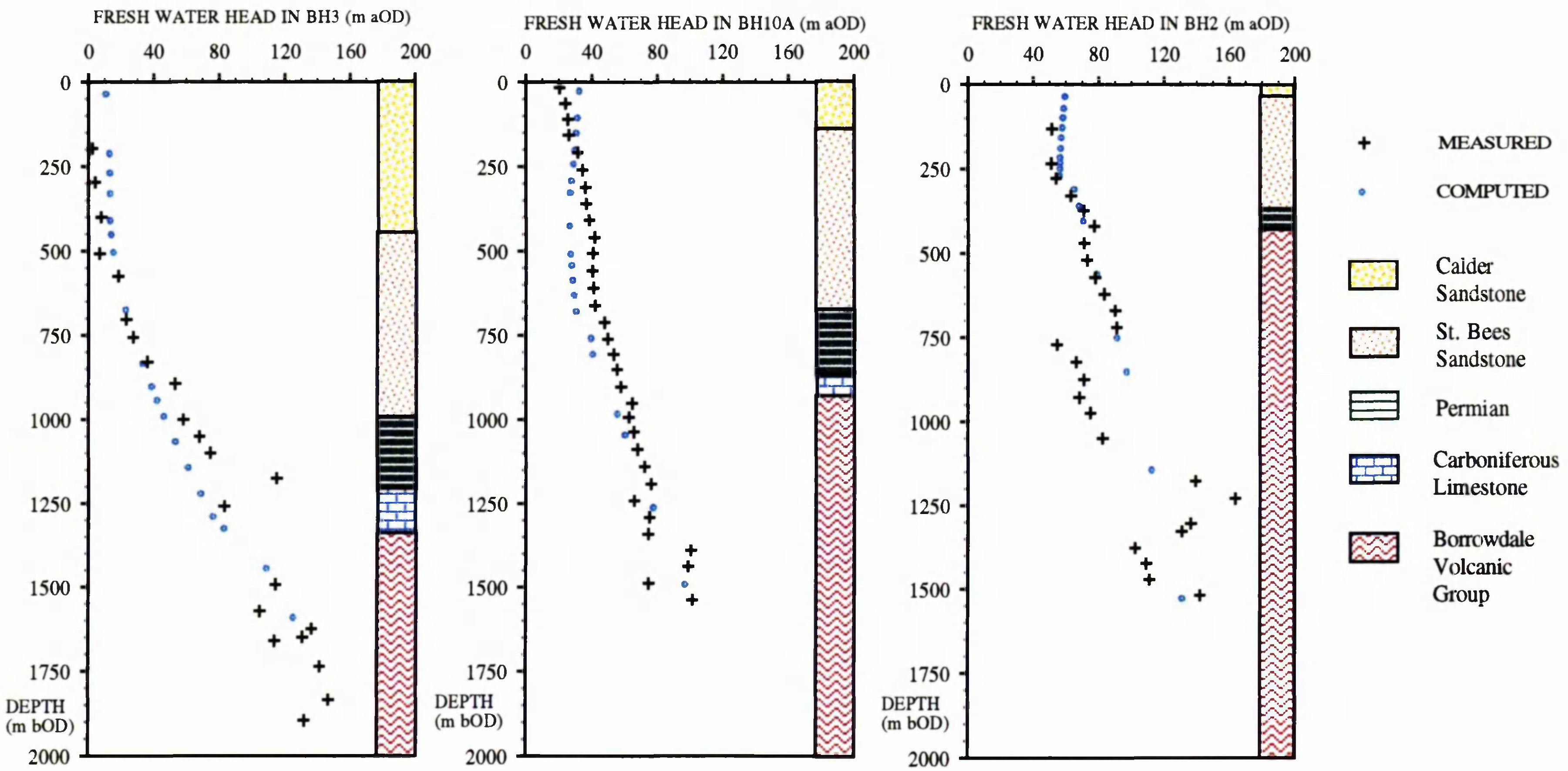


Figure 4-31 The computed head of the Seven-layer Model comparing in three boreholes

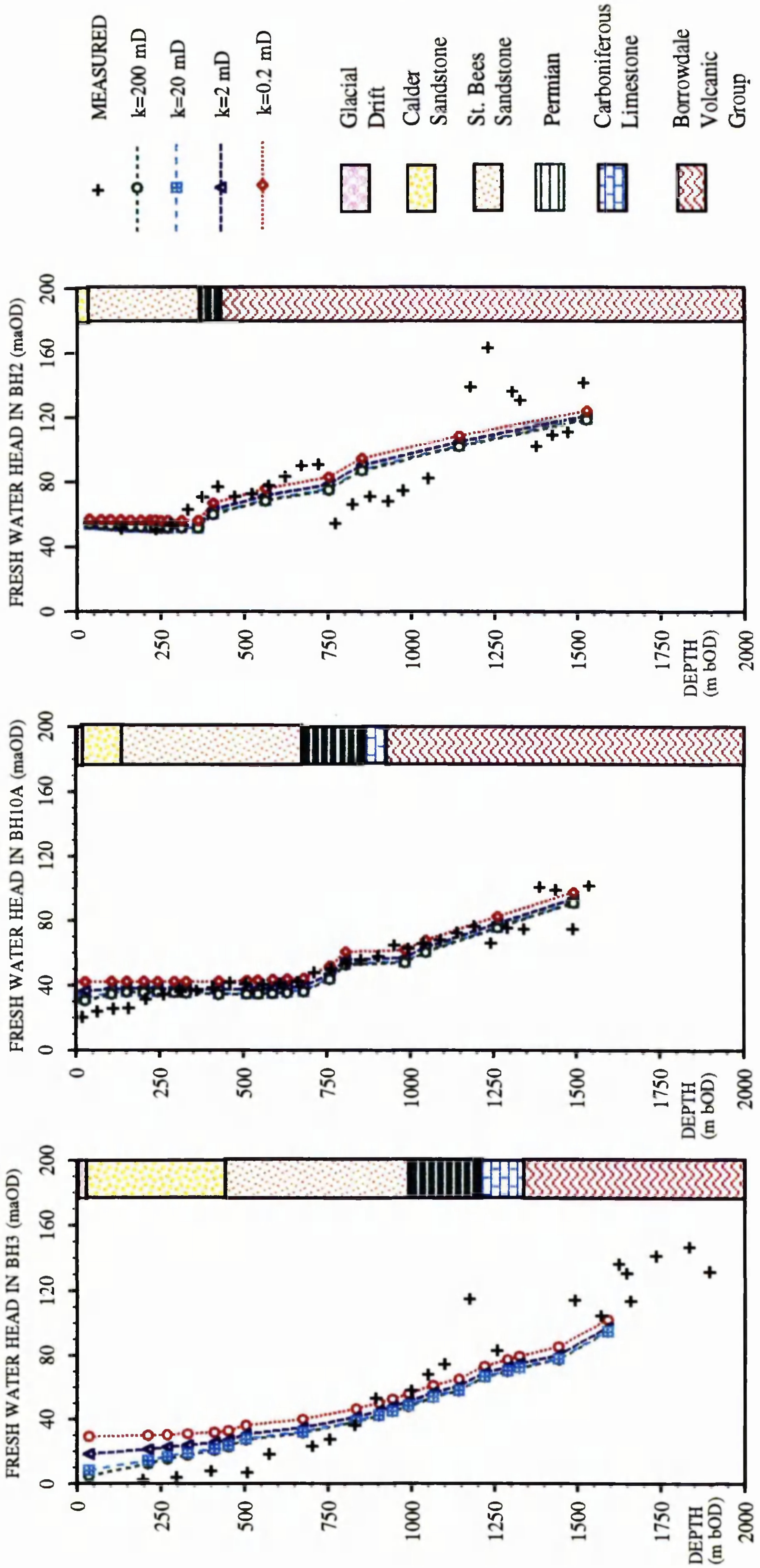


Figure 4-32 Sensitivity test of permeability on Glacial Drift in the Comprehensive Model

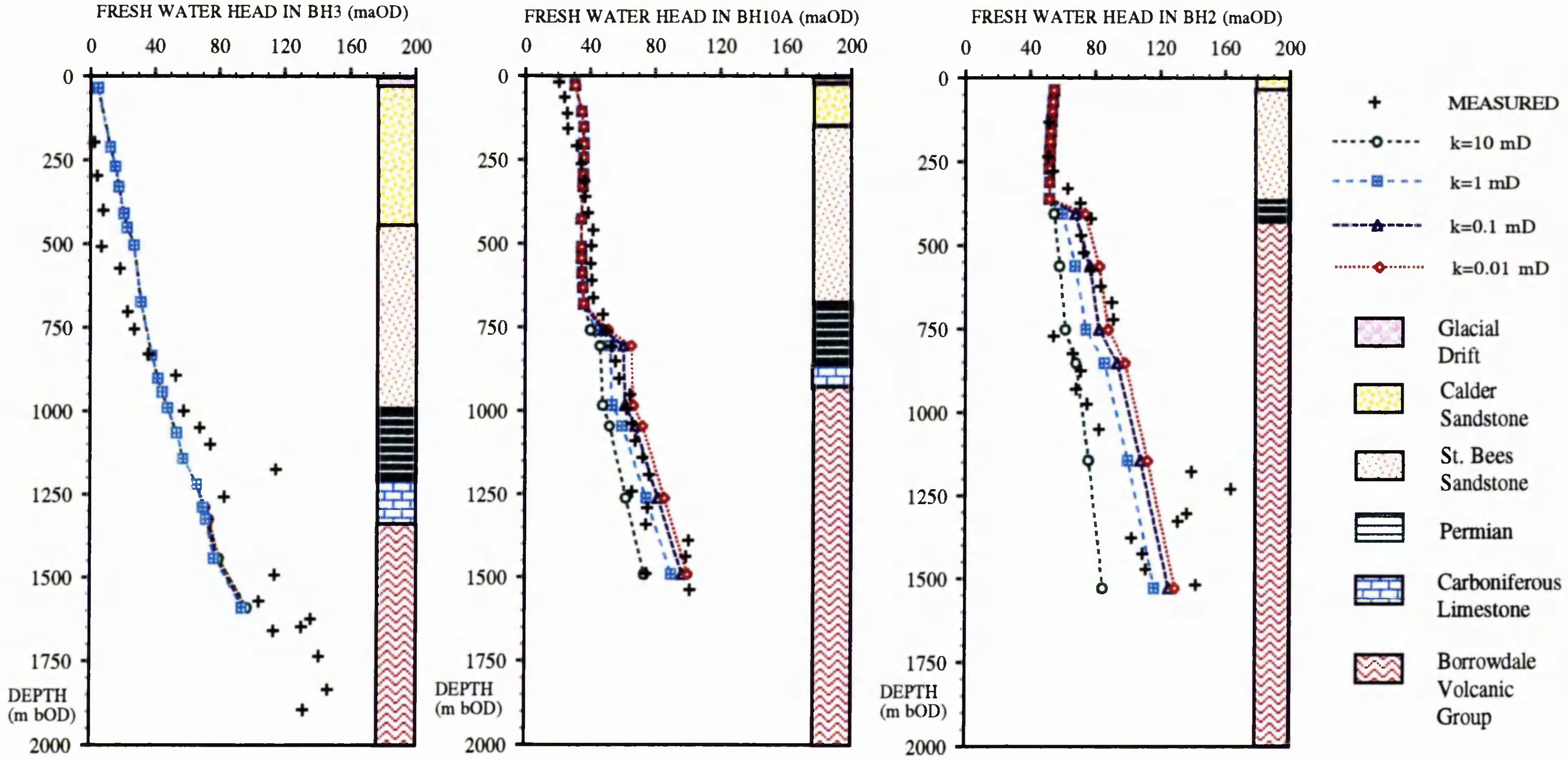


Figure 4-33 Sensitivity test of permeability on fault in the Comprehensive Model
The modelled head is very sensitive to the permeability of fault, both for BH10A and BH2

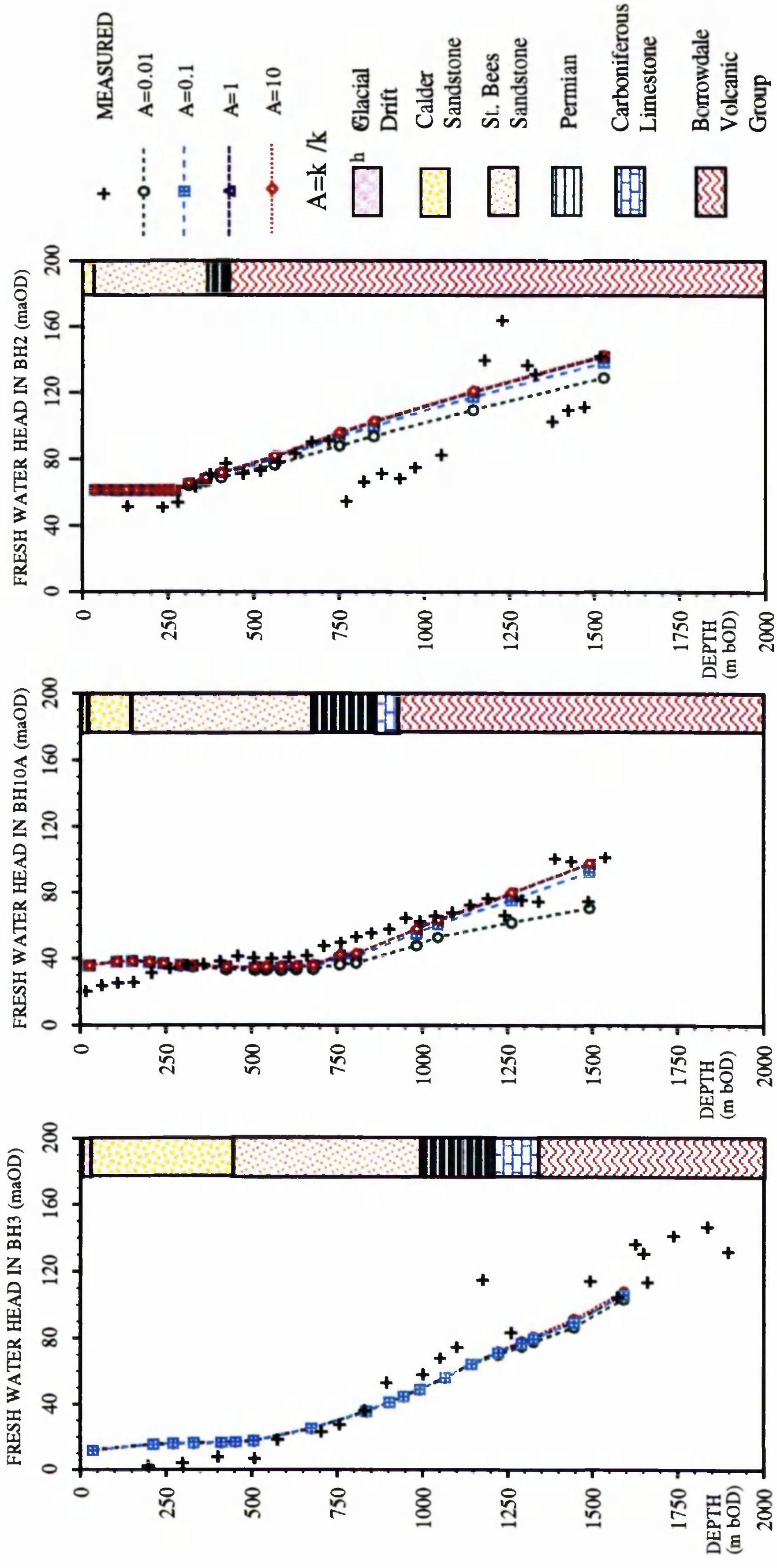


Figure 4-34 Sensitivity test of anisotropy on fault in the Comprehensive Model

The modelled head is also sensitive to the anisotropy of fault, in particular for BH10A

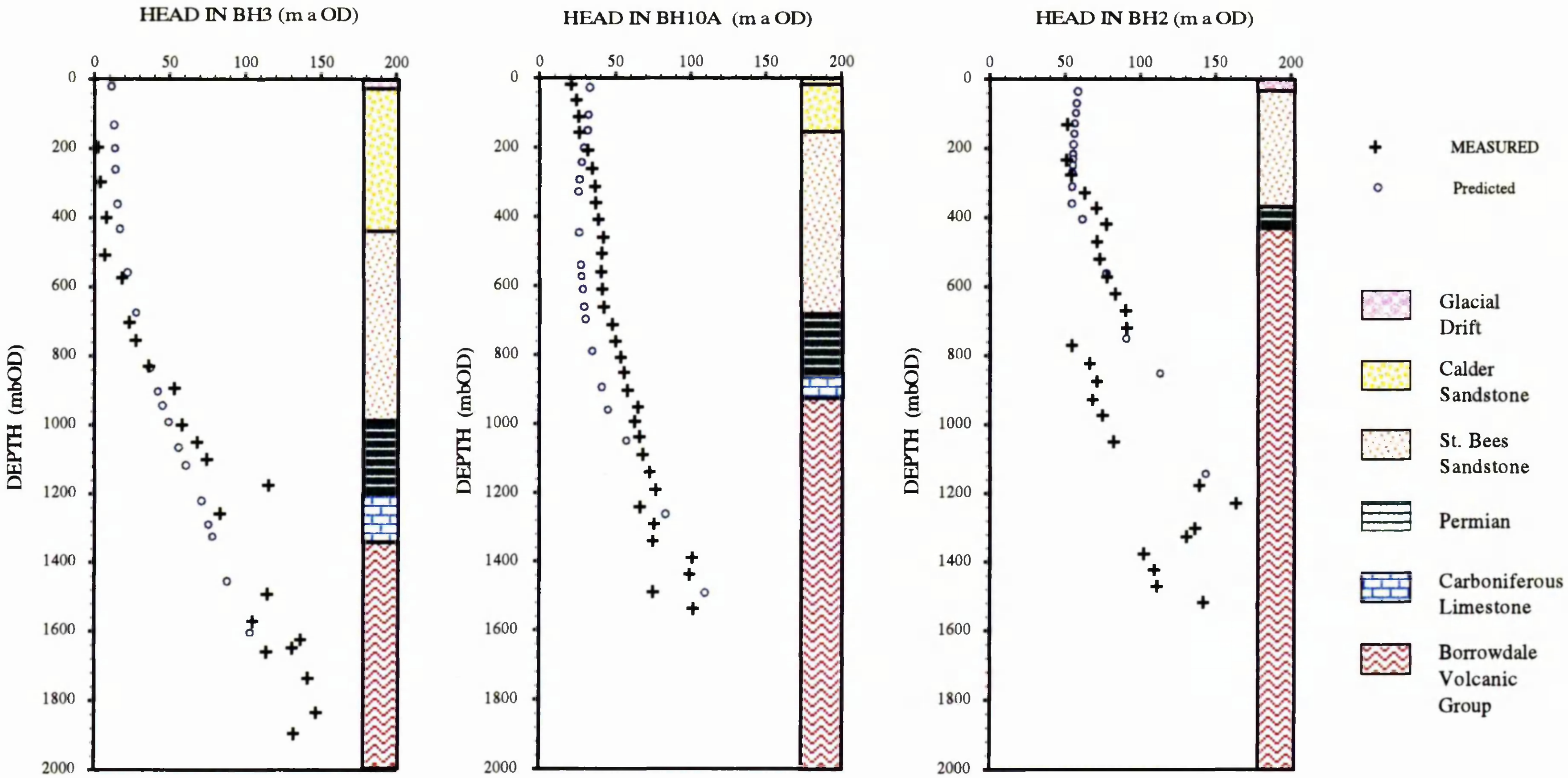


Figure 4-35 The modeled groundwater head from the Comprehensive Model
The predicted head is much closer to the measured one except in BH10A

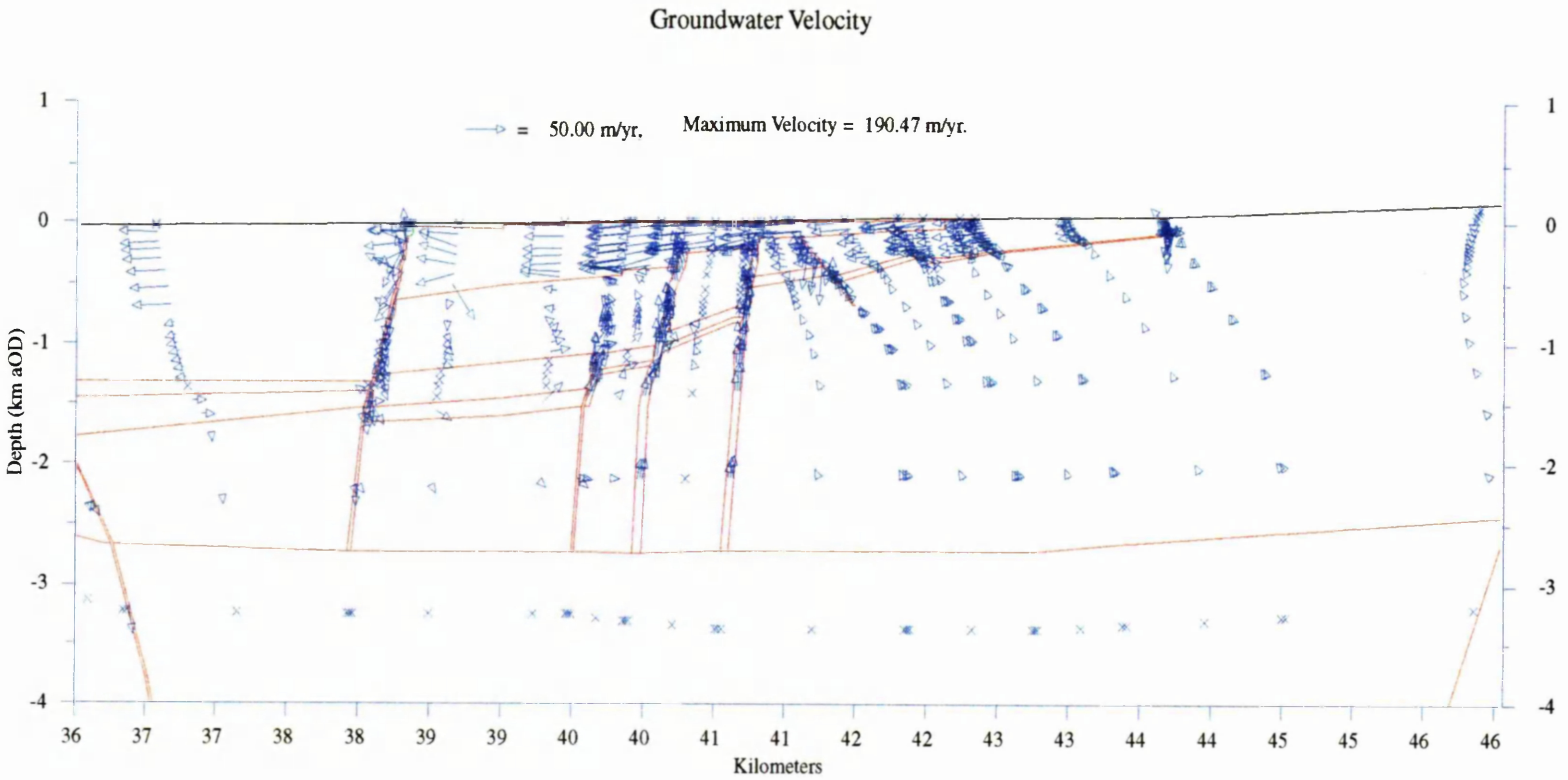


Figure 4-36 Groundwater velocity from the Comprehensive Model

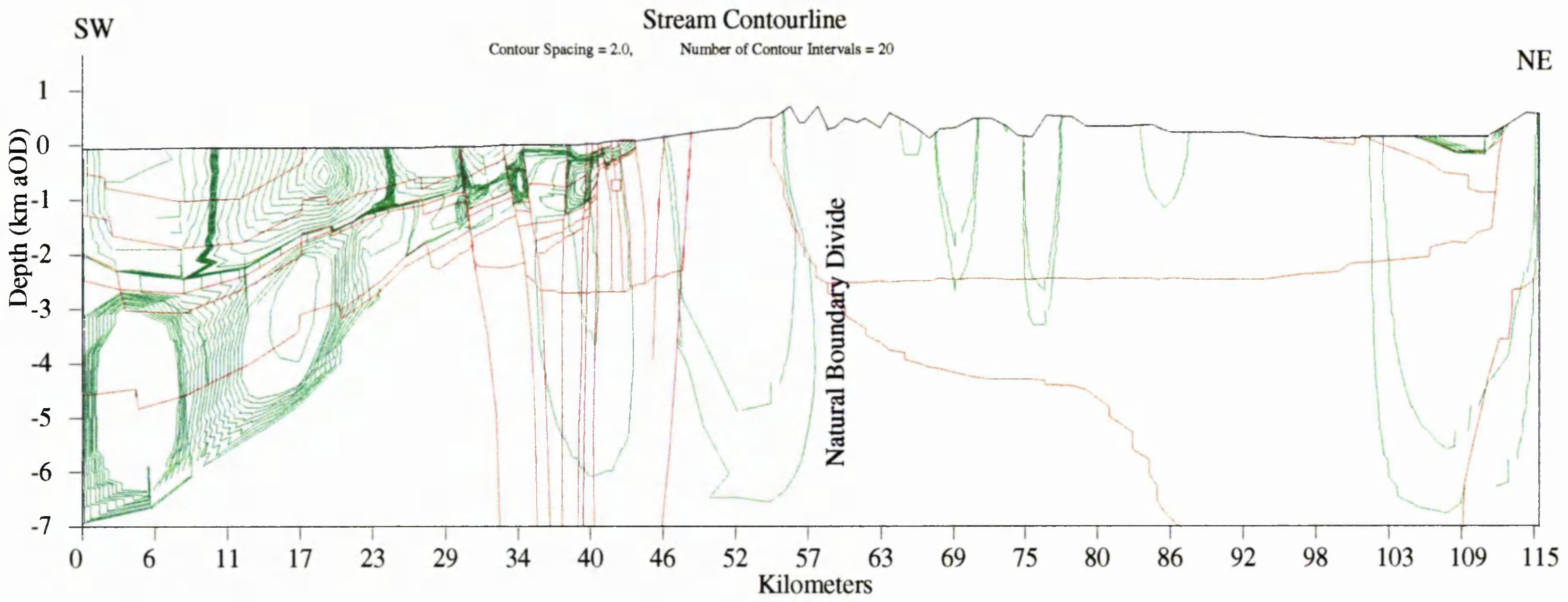


Figure 4-37 Stream contourlines from the Comprehensive Model

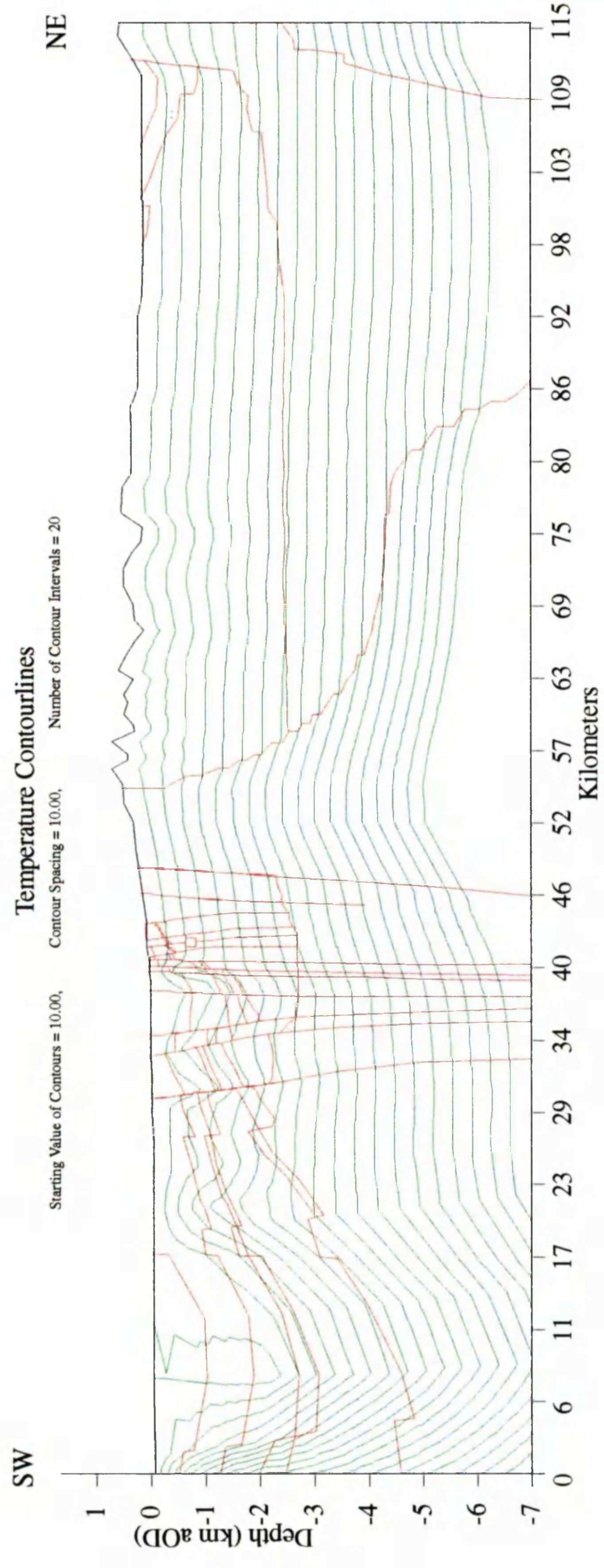


Figure 4-38 Temperature distribution from the Comprehensive Model

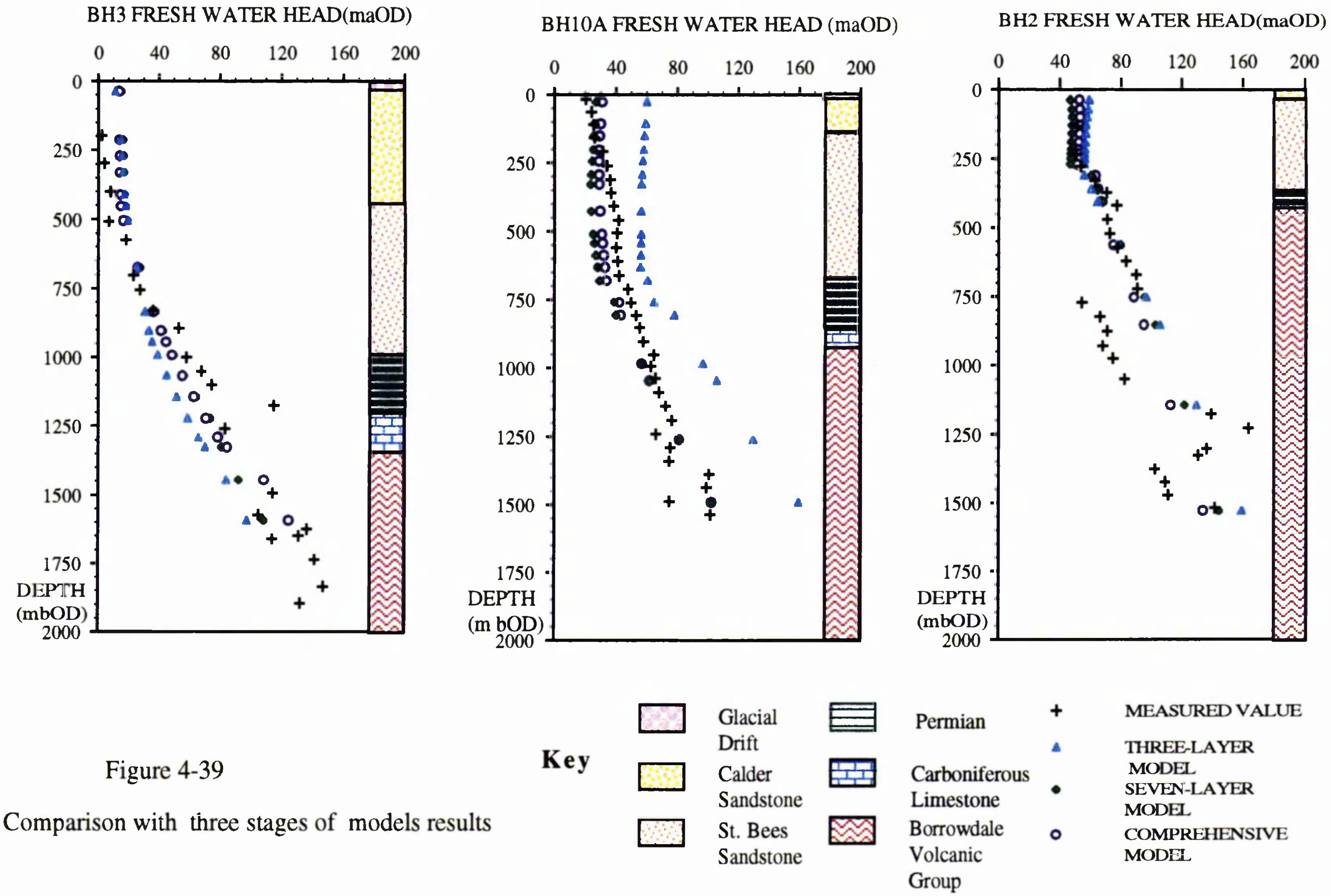


Figure 4-39

Comparison with three stages of models results

Chapter 5

MODIFICATION AND COMPARISON OF MODELS

1 INTRODUCTION

The groundwater flow represented by models is controlled by many factors, such as the type of the model, the concepts and assumptions, parameters fed into the model, the boundary conditions, and the discretisation of the elements. The use and the application of sensitivity tests and uncertainty analyses, in helping us to understand how good a match between model prediction and observations we can expect, was clearly demonstrated in the last chapter. In comparing results from experimental observations and model results it turned out to be difficult to determine how good an agreement could be expected, and how good a fit needed to be, in order to contribute to the building of confidence in the model. An experience from these former stages of modelling is that the more complex and well characterised the system being studied is, the better agreement is required between model predictions and observations of system behaviors. It is obvious from studying the results of those test cases that an increase in scale and complexity of the system, leads to a better fit between the model and the data. This is often with an attendant increase in the quality of characterization of the structure of the system, i.e.: the geometry, the geological structure, the type of the materials, and the boundary conditions, as well as the heterogeneity and anisotropy of materials.

As this model is used to simulate the regional groundwater flow system, it is possible that the mesh built for the model might be so coarse (because of computer size restrictions) that numerical dispersion could happen. Additionally, the measured data are constrained in a very small local area and this will inevitably cause differences when these locally measured data are extrapolated to a regional model because of rock heterogeneity. As was discussed before, the parameters are variable in space and it is not possible to express this variability precisely due to scarcity of data. As a result we are forced to make assumptions and inevitably this will involve bias. Some of these issues cannot be solved simply by using sensitivity tests. Therefore it is necessary to modify the models based on the factors which may cause unrealistic results, to enhance the accuracy of the model, which will in turn improve the confidence in the model. To achieve this, modifications were implemented in many respects: such as the heterogeneity of faults, the geometry of mesh representing the faults, boundary conditions, the minimum amount of elements needed in the regional model to avoid numerical dispersion. Emphasis was put on the modifications of faults that control the groundwater flow in the Borrowdale Volcanic Group, the density of the mesh in the local site and the boundary conditions.

At an early stage of modelling, concentration was put on reproducing the groundwater head at the repository site which was claimed to be difficult to simulate (NIREX, 1993). However, the groundwater head in BH2 can be easily reproduced simply by using the Seven-layer model in my regional modelling work. With the increase of understanding modelling groundwater flow in this area, it was realised that the best match of parameters fed in the model varies from borehole to borehole, this was not taken into account by the previous workers. For instance, the best fit in the Seven-layer model that matches the heads in BH3 and BH2 does not match those in BH10. A similar effect occurs in the comprehensive model. It also should be mentioned that the groundwater head in BH10, which lies between BH2 and BH3, has never been simulated or compared before this work. Yet it is found in this study that the heads in BH10 are actually the most difficult to reproduce. These are particularly studied in this chapter.

Since the results of the models vary from model to model, even using the same data in the same case, comparisons were made between my model and other published models (Heathcote *et al*, 1996). These take into account many factors such as the parameters fed into the model, boundary conditions, the conceptual model, in order to identify the reasons that cause the differences, and so enhance confidence in the model. One of the most effective comparisons was found to be when I extracted a district model that was the same size and location as the local model made by previous researchers. It could then easily be identified what the main differences are if the comparisons are made when identical conditions are set.

2 MODIFICATION OF THE MODEL

2.1 Modification of local mesh

The finite-element mesh was made up initially of 2300 nodal points. Among these, there were 800 nodal points to form the local mesh around Sellafield. It is likely that the regional model cannot accurately reproduce the local groundwater flow system if the mesh constructed is too coarse to represent the geological structures in detail. To reduce this impact, finer grids in the local area were required. We intensified the mesh in the Sellafield local area including the recharge area, until there was no significant effect from it. We found that the grids and elements were almost tripled to reproduce results of what it is expected, 2500 nodal points in the local area and 4000 nodal points in the total cross section. The modified grids and mesh are shown in Figure 5-1. Not only is the finer mesh necessary to improve the accuracy of groundwater flow modelling at Sellafield, but also it is needed to carry out nuclide transport simulations.

After having made the geometry modification, the sensitivity tests were repeated and consequently better results were obtained. The apparent consequences can be seen in Figure 5-2. The changes of results from the modifications are not only exhibited in improved matching heads, but also in velocity and other parameters as well. The maximum flow rate was down from 190m/yr to 36m/yr after reforming the geometry of the grids and mesh.

2.2 Modification of faults

In low permeability rocks the groundwater flow is concentrated in zones with an increased frequency of connected hydraulically conductive fractures. These fractured media usually have highly variable and uncertain permeable structures. Any leakage of radionuclides from an underground repository to the biosphere will presumably occur through such fracture zones. It is indicated by the investigation that the groundwater flows through the BVG are dominantly controlled by the fractures within it. The measurement of variable heads in the BVG of the Sellafield area is indicative of the large scale heterogeneity caused by this fracture network. Faults are also known to occur in the BVG, and the correlation between faulting and the flows needs to be understood. From the sensitivity tests in chapter 4, it was found that agreement between modelled heads and measured profiles cannot be achieved by simply adjusting parameters of lithologies fed into the model. That sensitivity testing also revealed the importance of faults in controlling groundwater flow at Sellafield. The groundwater flow must be fully understood by investigating features of these faults in the BVG. The features of the faults influencing groundwater flow were investigated separately, these included width, anisotropy, heterogeneity and conductivity.

Fault representation and scaling in flow models are examined in this model with respect to fault zone properties. Representation of a fault conflates the effects of four factors — fault zone thickness and permeability, grid-block size and matrix cell permeability. Ideally, one would like to represent the fractured rock mass and flow through it by models that accurately simulate the performance of each rock mass component. This is not possible, and all models are simplifications. These simplifications may be introduced in the form of continuum models, in which the discontinuum character of the rock mass is neglected, or in the form of discontinuum models which try to deterministically represent the discontinuities geometrically and mechanically. Our approach is using the latter form, which is the only acceptable form on such a regional scale. This scale of modelling has been proved to be successful through this study, in particular after the final stage of the modelling that is presented below.

2.2.1 *The width of faults*

The hydrogeological properties of faults and fractures were extensively tested during NIREX geological exploration. From the tests during drilling and post drilling, the hydrogeological information on faults and minor lithologies consists of inflow points from FSTs and hydraulic conductivity and head data from EPMs (NIREX, 1993). Not only does flow occur in the faults or fractures, but also the permeability of the faults varies from place to place. At an early stage of the modelling the initial width of the fault was set as 30 meters, to make it have a significant role in the groundwater flow system. However from statistics of field measurements (NIREX, 1993) only six of 18 fracture families appear to be closely related to faults. Faults (main plus minor) account for 36% of the flow zone structures. The larger flow zones tend to be associated with fracture families and minor faults. This implies that the fault zones should not be so wide as first presumed. Later fault widths were reduced to one meter, which results in a better match between modelled heads and real heads. This width is also in accordance with the field exploration and core log measurements.

When the width of the fault was reduced from 30 meters to 1 meter, there would be a numerical dispersion artifact resulting from the abrupt changes of mesh geometry. To avoid this a transition mesh was formed between the fault and the no-fault elements. The effect of this modification is shown in Figure 5-3.

2.2.2 *The heterogeneity of the faults*

The hydraulic conductivity of rocks varies from lithology to lithology, so does hydraulic conductivity in the faults. Heterogeneity of the faults was investigated with respect to the effects of four variables — fault zone thickness and permeability, grid-block size and matrix cell permeability. It can also be divided into two divisions: faults in sandstone; and faults in basement. The effect of heterogeneity of faults on the head pattern is significant. After a protracted investigation of fault heterogeneity, i.e., feeding various values of permeability parameters into the fault zone under the sensibility test until a better match between modelled heads and measured values was obtained. This was particularly true in BH 3, where a match was difficult to gain when the parameters of faults were set as uniform. The comparison of this achievement is presented in Figure 5-4.

The hydraulic conductivity of faults tends to be not far from the conductivity of the surrounding rocks, to ensure that the modelled groundwater head is consistent with the measured values. The certainty of test result is that faults in the Sandstone are apparently more permeable than those in the BVG. The hydraulic conductivity of faults in the sandstone is about two orders of magnitude higher than that of the BVG.

2.2.3 *The anisotropy of the faults*

The anisotropy of faults was investigated separately for two types of fault in sandstone and basement when they were treated as uniform. Using the sensitivity test, it was also found that the anisotropy of the faults varies with their lithology. Results of tests suggested that faults in the basement are more anisotropic than those in sandstone. All the results of sensitivity tests show that the vertical hydraulic conductivity of faults is higher than the horizontal, and this is quite reasonable because the faults in Sellafield are mostly vertical.

2.2.4 *The influence of faults on groundwater flow*

The widely spread distribution of faults in this area increases the complexity of the groundwater flow system, and results in the difficulty of simulation from scanty available data from the field. Although there are too many faults in the area to be fully understood using this model, still we obtained a few general characteristics of the groundwater flow in the faults or in their vicinity. Most of these characteristics are very important to understand.

Comparatively, the fault zone is more permeable than the surrounding rocks, the hydraulic conductivity of faults is about one order magnitude higher than that of the surrounding rocks. So, consequently, is the flow rate as well.

2.3 Modification of Boundary

The hydraulic interference tests were predicted based on limited information, where transmisivity values were primarily obtained from limited borehole measurements and the boundary conditions were simplified. The outcome of the tests showed that the predictions of the model did not describe the flow field satisfactorily. Thus boundary conditions were revised by adding more recent geological interpretations, and the inverse modelling from the interference test was carried out. The inverse modelling generally verified the updated boundary conditions, and the interference tests could be simulated relatively well.

The initial code of OILGEN assumes that the groundwater table follows the topography. This also might be one of the reasons that cause a mismatch in the upper groundwater table. A modified version of OILGEN software reset the groundwater table according to its location, i.e. whether it is near to the sea or on the mountain. All the nodal points west of the coast are set at a constant head equivalent to sea level. The others inland are set 0 to 5 meters below the land surface.

3 THE RESULT OF THE MODIFIED MODEL

3.1 Sensitivity test

The parameters used in the model were retested after the model was modified. The result of the re-test is given in Table 5-1. During previous stages of modelling, the best fits of parameters are not unique. Among these sets, each suite of parameters can be one order magnitude higher or lower systematically at the same time. It is suggested that the comparative permeability is also one of the main factors controlling groundwater head pattern. Through all the progressive testing, an important result that has been sought is a unique result for a combination of best fit parameters. In other words, the uncertainties that existed in previous models are progressively eliminated after more complicated conditions were simulated, with better quality of the characterization of these materials. After the modification of relevant factors there is only one suite of parameters among those several sets of parameters used to fit the earlier models which still keeps a good fit. The phenomenon is illustrated in Figure 5-5, which presents the comparison between the best fit parameters and the other sets which are one order magnitude less, or more, than the best fit.

3.2 Flow pattern

The groundwater flow patterns are dependent on the hydraulic properties of geological materials, the geological structure in the research area, the salinity distribution in the groundwater, thermal properties of the rocks, and so on. All these uncertainties are progressively narrowed or reduced using the available data at different stages. The most important point is that the best fit parameters that reproduce the best match between modelled head and measured head in the boreholes are unique rather than uncertain. On the other hand, with the development of complexity and well characterization of the system being studied, a better agreement is obtained between model predictions and observations of system behavior. It is obvious from studying the results of these test cases that a satisfactory result has been gained after the last modification of the model. Indications of the groundwater flow feature can be discussed below.

3.2.1 *Freshwater head*

The freshwater head contour along the cross section is drawn to show the flow pattern of groundwater at Sellafield (Figure 5-6). The goodness of fit of the modelled flow pattern can also be assessed based on the freshwater head contour, and this is more clearly displayed. Both the predicted groundwater contours, and the measured ones based on three boreholes, are drawn in Figure 5-6. It can be seen that the pattern of modelled contours is quite similar to the measured one, except in far east where the modelled value is lower than that measured by NIREX. From the groundwater head contour map it is suggested that groundwater flow in a horizontal direction is very slow because the horizontal space of the contour lines is rather significant, which implies a smaller hydraulic gradient occurring in this area.

3.2.2 *Groundwater velocity*

The groundwater flow field can be explicitly displayed by the flow vector diagram, which is presented in Figure 5-7. All the flow in this area dominantly occurs above the depth of -1,700 meters OD. The general feature of the regional groundwater flow system is that the fastest flows are in the superficial sandstones and the BVG at Sellafield. The slower flow system, less than 1 m/yr, is in the east. A static flow system exists 1.7 km below OD. The fastest flows are in the St Bees Sandstone Group and adjacent Borrowdale Volcanic Group. It should be noted that the flow rate in the BVG where the repository site would be located is faster than originally supposed, about 0.8 m/yr. This is also the reason why the fresh water head is higher than those modelled ones. The high pressure within the area of BH 10A can only be reproduced by setting the hydraulic conductivity of the BVG one order of magnitude higher than the median field-measured values. In the limestone there is also another faster flow zone that can be distinguished from other lithologies. It is of interest that the higher flow rates do not necessarily happen in the more permeable rocks. Instead, rapid flows exist in the low permeability rocks of the BVG, these could result from the distribution features of the BVG recharge and discharge areas, and the subsurface flow path as well.

3.2.2 *Groundwater recharge and discharge*

The groundwater recharge and discharge at Sellafield, in particular the deep underground water flow system, are well simulated by the regional model. The general features can be explicitly displayed in the streamlines (Figure 5-8). It can be seen that the eastern part of the area, land and hill, is the recharge area; and the west area, the East Irish Sea, is the discharge area. The groundwater is recharged from precipitation, which percolates into the subsurface and flows east towards the coast. Most water flows superficially, some of it percolates deep underground, takes a long journey across the repository site (the rectangle on the map) and then to the offshore. The denser lines in the western shallow area suggest that most of the groundwater flux is in the shallow Sandstone Group. There is an almost no flow area in the west from the PRZ below 1.7 km OD.

3.2.4 *Groundwater flow regime division*

The groundwater flow route and flux rate can be well depicted by the stream line contours. There are significant differences within these stream line contours, based on which the groundwater flow regime can be divided into three parts. Firstly, in the shallow Sandstone Groups of the western area, there are dense streamlines that mean greater water flux, this is called the Shallow Water Regime. Secondly, to the east of the coast, the stream lines are sparse because of less water flux, this forms the Inland Groundwater Regime. The last, is the deep East Irish Sea Basin below -1.0 km OD, where there is almost no flux except for free convection resulting from variations of salinity; this is termed the East Irish Sea Basin Regime.

The stream lines obtained from the model clearly reveal the characteristics of the subsurface groundwater flow. This agrees very well with the conceptual model based on hydrogeological data. Borehole 2, where the repository site was proposed to be located, is in the west end of the Inland Groundwater Regime. The sources of salinity in BH2 could come from the east and result from the water-rock reactions in the BVG. In contrast, Borehole 3 is in the East Irish Sea Basin Regime. The ratio of Br/Cl in Borehole 3 is lower than in that Borehole 2 (NIREX, 1993), and its source may be the evaporites of the East Irish Sea Basin Regime. The Br/Cl ratios for saline groundwaters and brines in Borehole 3 have a constant Na/Cl ratio (ca 0.66 by mass), with increasing salinity whereas the saline waters in the BVG from Borehole 2 show a trend of decrease. This trend in the BVG could also be interpreted as a result of progressive water-rock reaction within the BVG which depletes Na during the long distance of travel. The stream line contour map shows the route of groundwater from precipitation in the inland hill area, then going deep underground and starting its long journey towards the coast. During this long time of travel, the salinity could have accumulated due to water-rock interaction.

3.3 Temperature distribution

The temperature distribution from the modified model is shown in Figure 5-10. There is not much change in the temperature after the modification of the regional model, except to produce smoother contour lines because of lower flux.

3.4 Conclusion

After progressive modification of the model, the following conclusions can be drawn:

(1) The size and geometry of the model is very important in the numerical model. In particular, when modelling the regional scale groundwater flow, a numerical dispersion can be produced if the mesh of the grids is too coarse.

(2) The improvement from modifying the model is very significant and the modified model can reproduce all the measured freshwater heads in boreholes 3, 10A, and 2. In other words, the modified regional model result can represent the real local groundwater flow system at Sellafield.

(3) The simulation is also very sensitive to the geometry of the mesh used to simulate faults. This suggests that the width of faults used in the model should be as consistent as possible with their real width.

(4) Anisotropy and heterogeneity prevail in all the types of rocks at Sellafield, which strongly influence the flow pattern and flow rate.

(5) The groundwater flow regime can be divided into three parts. The Shallow Water Regime, distributed in the Sandstone Groups on the coast and offshore, the Inland Groundwater Regime, distributed in the eastern land and hill area and, lastly, in the deep East Irish Sea Basin below (-1.5 km OD), where there is almost no flux except free convection resulting from the variance of salinity, termed the East Irish Sea Basin Regime.

(5) The eastern part of the land and hill area, the Inland Groundwater Regime, is the recharge area. The groundwater is recharged from precipitation, percolates into the subsurface and flows towards the west. The upper west area, the Shallow Water Regime, is the dominant flow area. The ground water flow focuses into this area due to higher permeability sandstone, and discharges towards the offshore. Most water flows superficially. The deeper western area, the East Irish Sea Basin regime, is almost a non-flux area.

4 COMPARISONS OF VARIOUS MODELS

4.1 Introduction

Modelling groundwater flow at Sellafield began in 1992 (Heathcote *et al*, 1996) and was done by a number of organizations. It was primarily integrated by Heathcote (1996), then Stuart Haszeldine and Christopher McKeown (McKeown *et al*, 1999). It was found that the result of the modelling varied from model to model. To find out what caused the differences and why previous workers failed to reproduce ground water head in modelling, I made comparisons between these models. Differences included the boundary conditions between my regional model and their local models, hydrogeological parameters used in models, geometry of the mesh and grids, and the basic conceptual model as well. This new work will also help to increase confidence in the model. To achieve this we extracted a district model that is the same size and location as models used by previous researchers. It can then easily be identified what the main differences are if the comparisons are made when the same conditions are set.

The main objective of NIREX modelling was to help develop a conceptual understanding of the hydrogeology. They constructed four groups of models, but only the two-dimensional vertical section models incorporated the BVG and salinity which are vital for modelling groundwater flow at the repository site. The vertical section modelling in NIREX work (NIREX, 1993) was intended to test the concept of fresh water flow from the hills being in dynamic equilibrium with saline flow from the East Irish Sea Basin. The two-dimensional vertical section is 12.5 km long and 2.5 km deep, constructed in a idealised section (Figure 5-11) using the finite element code SUTRA (Gorelick *et al*, 1984). The eastern vertical boundary, close to the watershed, and the bottom boundary, were taken to be no-flow boundaries. The top boundary is a fixed head boundary equivalent to the ground surface onshore, and to the sea bed offshore. The parameters used in the model are given in Table 5.2. There was no calibration of this modelling. The heads predicted by the model only agree with those in Borehole 3. The model does not explain the observed head in Borehole 2 and the salinity of the eastern source of the saline water (NIREX, 1993). The heads between Borehole 3 and Borehole 2 were not considered in this work. The model ran in transient mode, starting with the system full of fresh water to establish a base case. Pseudo equilibrium was reached after 10^8 years. A steady-state model was developed using NAMMU finite-element code to investigate the dispersion required to match the observed saline transition zone (NIREX, 1993).

Christopher McKeown constructed a similar cross section to that of NIREX, about 14 km long and 2.5 km deep (Haszeldine & McKeown, 1995; McKeown, 1997). To discretise the study area, 2204 nodal points and 4200 elements were used (Figure 5-12). The conceptual model of McKeown builds on the conceptual model of NIREX, i.e., the groundwater at Sellafield is gravity driven, moving in a generally SW direction from the uplands of the Lake District through the PRZ towards the Irish Sea, where the brines might act as inhibitors to the flow of groundwater. The boundary conditions are the same as NIREX's. The aim of his model was to predict the date when radioactive waste could return to the surface. His model was run using the OILGEN code to compute the groundwater flow and radio-active waste transportation. The result of the modelling was assessed using Borehole 2 and Borehole 3. There was no consideration of matching heads in Borehole 10 in his study. The comparison of in-situ fresh water head with that calculated from the model indicated that the best fit simulations had to set the BVG hydraulic conductivity to 1.2 m/yr, which is 2 orders of magnitude higher than the median field value. It was concluded that the best fit is not affected by the variation in hydraulic conductivity of faults. The hydraulic conductivity of the St Bees Sandstone, the Permian, or of faults, is not important to the repository flow rate and the median conductivity values of these overlying sediments also have good fit (McKeown, 1997).

4.2 The District Model

4.2.1 *Concept of the model*

The district model was abstracted from the regional model, it was 14 km long and 2.5 km deep, and about the same location and size as the models mentioned before. 2125 nodal points and 4032 elements were used in the district model (Figure 5-13). The objective of this model was to characterise the groundwater flow on the small scale, focusing the investigation onto flow patterns in the Sellafield district area, evaluating scale effects on modelling groundwater flow. Most importantly, this district model will make comparisons between models from various workers and identify the main reasons which produce differences, and so enhance the confidence of the modelling.

Similar to the models made by others, the vertical and bottom boundaries of this district model are set to be no-flow boundaries. The top boundary is a fixed head boundary equivalent to the ground surface onshore, and to the sea level offshore. All the calculation in the district model was carried out by the modified OILGEN code.

4.2.2 *Parameters input*

The base case of the model was assigned using best fit input parameters (Table 5.1). The other sets of the parameters from the regional model (Table 5.2) used by NIREX and by McKeown are also tested in this model to analyse the differences due to the variety of the models. All these tests were carried out separately and independently.

4.2.3 *Results from the district model*

Results from the district model are presented by means of a section showing freshwater head, velocity field, streamline and temperature distribution. The modelled water head was compared to the measured head plotted against depth and the goodness of fit of the results can be seen in Figure 5-14. It was no surprise to find that the predicted head is much lower than measured values, which is the same as NIREX discovered using their models. The trend of this difference is that the more western the location, the lower the predicted head. This phenomenon can also be seen in the water head contours. The fresh water head from the district model is represented in Figure 5-15, in which the fresh water contour line is much sparser than that in the regional model (Figure 5-6).

As the water head is lower than the real values, so is the water velocity. From the velocity diagram (Figure 5-16), it is shown that the water velocity in the district model is much lower than the regional model. The other significant phenomenon in this model is that there is a local convection near the repository site, which is shown in the stream lines (Figure 5-18). This is the same as McKeown's model (McKeown, 1997).

4.3 The comparisons among the models

Although there are general similarities among these model simulations which all show that groundwater flows from eastern areas towards the offshore, if we look at the detailed results from fresh water head, velocity field and stream lines, there are apparent differences between the district model and the regional model. In contrast, there are lots of similarities among the various district models from different workers.

4.3.1 *Freshwater head*

It is not surprising that the groundwater head from the district model as well as the local models from other workers did not match the measured values at the location of Borehole 2. It should be noted that the eastern part is much worse than the western part. This implies that there is something missing on the eastern boundary. Figure 5-14 shows that the differences between the district model and the regional get higher from Borehole 3 in the west to Borehole 2 in the east. The fresh water head contours also show the same result in cross section (see Figure 5-18, Figure 5-19).

In order to raise the modelled groundwater head in BH2, we increased the value of hydraulic conductivity in the BVG just as McKeown did in his model. It is not surprising that the water head is much higher after that. That might explain why the hydraulic conductivity of the BVG in McKeown's model is about two orders of magnitude higher than the NIREX value (McKeown, 1997), and one order of magnitude higher than the median field value. However, the head in BH10 is still not reproduced by doing this (Figure 5-17). Despite the head match in BH2, there are still many differences of flow pattern between the local model and the regional model, which are discussed below.

4.3.2 *Groundwater flow velocity*

The differences in flow pattern between the local model and regional model can be deduced by comparing the diagram of distinct groundwater flow velocity (Figure 5-16) with that of regional flow velocity (Figure 5-7). Because of the lesser gradient of groundwater head resulting from the lower head in the east, the groundwater flow rate in the BVG where the proposed repository site was to be located is greatly reduced, from about 1 m/yr in the regional model to 0.1 m/yr in the district model. This will directly impact on the prediction of the migration of the radioactive waste leachate from the disposal site. Meanwhile, the flow rate in the St Bees Sandstone is comparatively higher in this case.

4.3.3 *Streamline contours*

The streamline contours (Figure 5-18, 5-19) also show a significant difference between the Regional Model and the District Model. Both of the models were input with the same hydraulic parameters, the streamline contours from the Regional Model show a lot of stream lines in the east (the right side of the PRZ). In contrast, there are very few stream lines in the east in the District Model. This result shows that there is little water influx from the east part of the land and hill area in this district model, although the hydraulic conductivities input in the District Model were the same as those in the Regional Model. This shows that recharge from the coast in the District Model is much less than that in the Regional Model. The reason for this lesser recharge from the east is the assumption of a no-flow boundary as the eastern vertical boundary. This result tells us that the low permeability rocks play a very important part in the deep underground water flow system. These deep flows are always very low compared to the higher permeable shallow aquifer systems, but these should not be neglected in studying low permeability rocks.

These models have been compared in many respects, such as fresh water head, groundwater contours, streamline contours and groundwater flow field. From this it is identified that the main reason why the fresh water head obtained from a local model is below the measured value, is because the main lateral recharge from the low permeability rocks is neglected.

4.4 Conclusion

Through the comparison of these models in many respects, the following conclusions can be drawn:

— The Regional Model simulates the groundwater system better than the local models at Sellafield, both in reproducing the measured groundwater head and the recharge area.

— There are many differences between modelling results from the Regional Model and those of the District Model. These differences can be displayed through the head pattern, water flow velocity and water flux.

— There are general similarities among previously published local models and the district model. The same result can be obtained if the same conditions are set.

— There are no obvious scale effects on the Regional Model, the best fit parameters in the regional model are close to the field median permeability values measured in-situ.

— The reason why the fresh water head obtained from the local model was below the measured value, is that the recharge from the low permeability rocks is neglected. i.e., the eastern vertical boundary should not be treated as a no-flow boundary in the local models.

—The groundwater head obtained from local models in BH2 can be raised by setting higher hydraulic conductivity in the BVG, but this cannot explain the head in BH10. Consequently, the flow pattern obtained cannot accurately represent the actual system.

— The low permeability rocks play a very important part in the deep underground water flow system, even though these flows are less than shallow aquifers. Hence, they should not be neglected in modelling low permeability rocks.

—The groundwater head was affected by restrictions of the local model. Consequently the groundwater flow rate in the BVG where the proposed repository site is located was influenced as well. The regional modelling results suggest that the flow rate in the PRZ is about 1.0 m/yr, where the district model predicts much slower flows of 0.1 m/yr.

5 SUMMARY

From previous stages of modelling it is suggested that the more complex and well characterised the system being studied is, the better agreement is achieved between model predictions and observations of system behavior. It is obvious from studying the modelling that an increase in scale and complexity of the system leads to a better fit between the model and the data. This is often with an attendant increase in the quality of characterisation of the structure of the system, i.e., the geometry, boundary conditions, and the heterogeneity and anisotropy of materials.

Because of the limitation of the computer memory, it is likely that element construction in the regional model is so coarse that numerical dispersion could happen. If this was so, the regional mesh could not reproduce accurately the local groundwater flow system if the mesh constructed is too coarse to represent the geological structures in detail. To reduce these impacts, it is necessary to modify the model both geometrically and conceptually. The improvement by modifying the model is very significant in this study and the modified model can reproduce all the three boreholes' measured freshwater heads. In other words, the modified model can adequately represent the real groundwater flow system at Sellafield, both at local size and at regional size.

The regional model clearly reveals the basic features of the regional groundwater flow systems, which have never been studied before. The east part of the area, land and hill, is the recharge area; and the upper west area, the East Irish Sea, is the discharge area. The groundwater is recharged from precipitation, percolates into the subsurface, and flows east towards the coast. Most of the water flows superficially. The deeper western area is almost a non-flux area. It should be noted that groundwater flows through the PRZ is recharged laterally from precipitation in the mountain area, and this percolates into the deep subsurface, and takes a long journey across the repository site (Figure 5-8) to the offshore. Based on the results of modelling, the groundwater flow regime can be divided into three parts: the Shallow Water Regime, distributed in the Sandstone Groups on the coast and off shore; secondly, the Inland Groundwater Regime, distributed in the eastern land and hill area; thirdly, in the deep East Irish Sea Basin under -1.5 km OD, where there is almost no flux except free convection resulting from the variance of salinity, this is termed as East Irish Sea Basin Regime.

The regional modelling also shows that there are two possible sources of salinity, one is the East Irish Sea Basin Regime, from halite rocks. The other is the Inland Groundwater Regime, from the water-rock interaction during the long time and long distance of traveling.

Since the results of modelling vary from model to model, it is necessary to find reasons causing these differences and to build confidence in the modelling. Comparisons can only be made when identical conditions are set. Through the comparison of these models in many respects, such as fresh water head, groundwater contours, streamline contours and groundwater flow field, the main reasons why the results of the regional model are different from the local model are determined. The same results were obtained in my district model as NIREX achieved using their models. In comparing McKeown's model with my district model, the very high hydraulic conductivity of the BVG obtained from McKeown's work was also reproduced this time. However, this high value did not match the head in BH10, which was not involved in his work. The important thing is that although the freshwater head in BH2 can be reproduced in a local model by input of very high hydraulic conductivities of the BVG, this could not reproduce the total local flow system with respect to either flow velocity or flow path, and this will inevitably influence the prediction of the safety of the proposed repository site.

The low permeability rocks take a very important part in the deep underground water flow system, even though flow is always negligible compared to the higher permeable shallow aquifer systems. However, deep flow should not be neglected in dealing with low permeability rocks. The importance of low permeability rock in regional deep groundwater flow systems has been proved in this study. The reason why the NIREX prediction of fresh water head in their local model was below the measured value is that the recharge from low permeability rocks was neglected, i.e., the eastern vertical boundary should not be treated as a no-flow boundary in the local models.

Not only was the groundwater head affected by the restrictions of the local model, but also the groundwater flow rate in the BVG in which the proposed repository site locates was apparently influenced as well. The regional modelling result suggested that the flow rate in the PRZ was about 1.0 m/yr, where the local model predicted 0.1 m/yr flow rate. This will directly affect the prediction of the safety of the proposed repository site.

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Permeability K (millidarcy)	**Drift**	**Calder Sandstone**	**St Bees Sandstone**	**Permian**	**Carbonife-rous Limestone**	**BVG**
Median Field Value		10	3	0.06	5	0.01
Regional Model	10	10	3	0.004	4	0.4

Table 5.1 The best fit permeability values in the Modified Model

Hydraulic conductivity (m/yr)	**Drift**	**Calder Sandstone**	**St Bees Sandstone**	**Permian**	**Carbonife-rous Limestone**	**BVG**
NIREX Value	180-373	109	31 - 108	0.003	0.3	0.0005 - 0.1
McKeown's Value		3	0.42	0.0001	0.15	1.2
My models's Value	3	3	0.93	0.0012	1.24	0.12

Table 5.2 Horizontal hydraulic conductivity values used in NIREX AND McKeown 's models

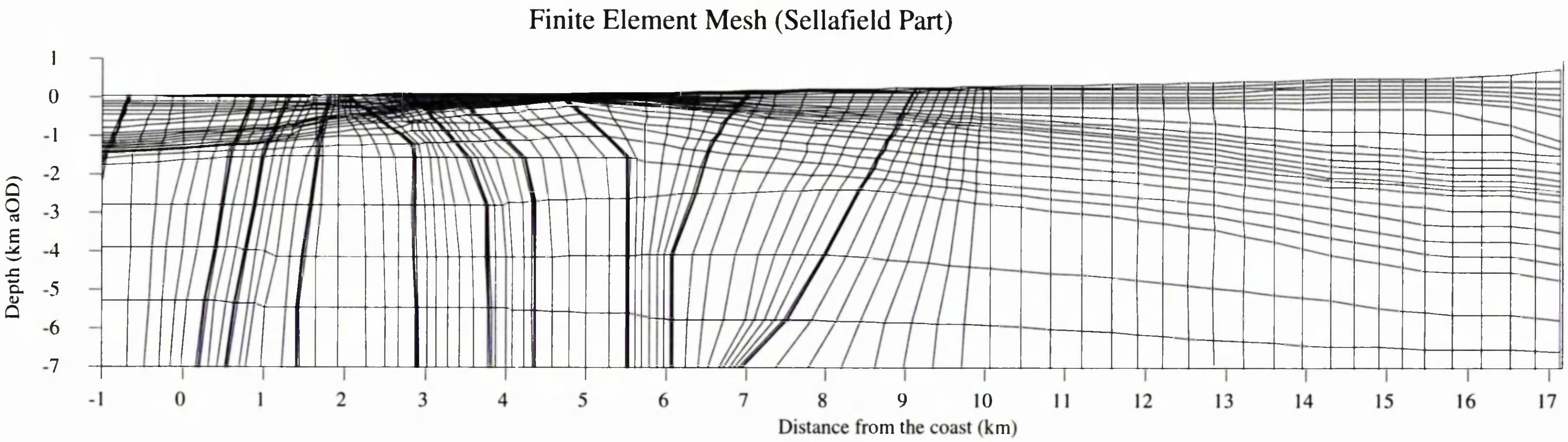


Figure 5-1 Quadrilaterals used in modified models

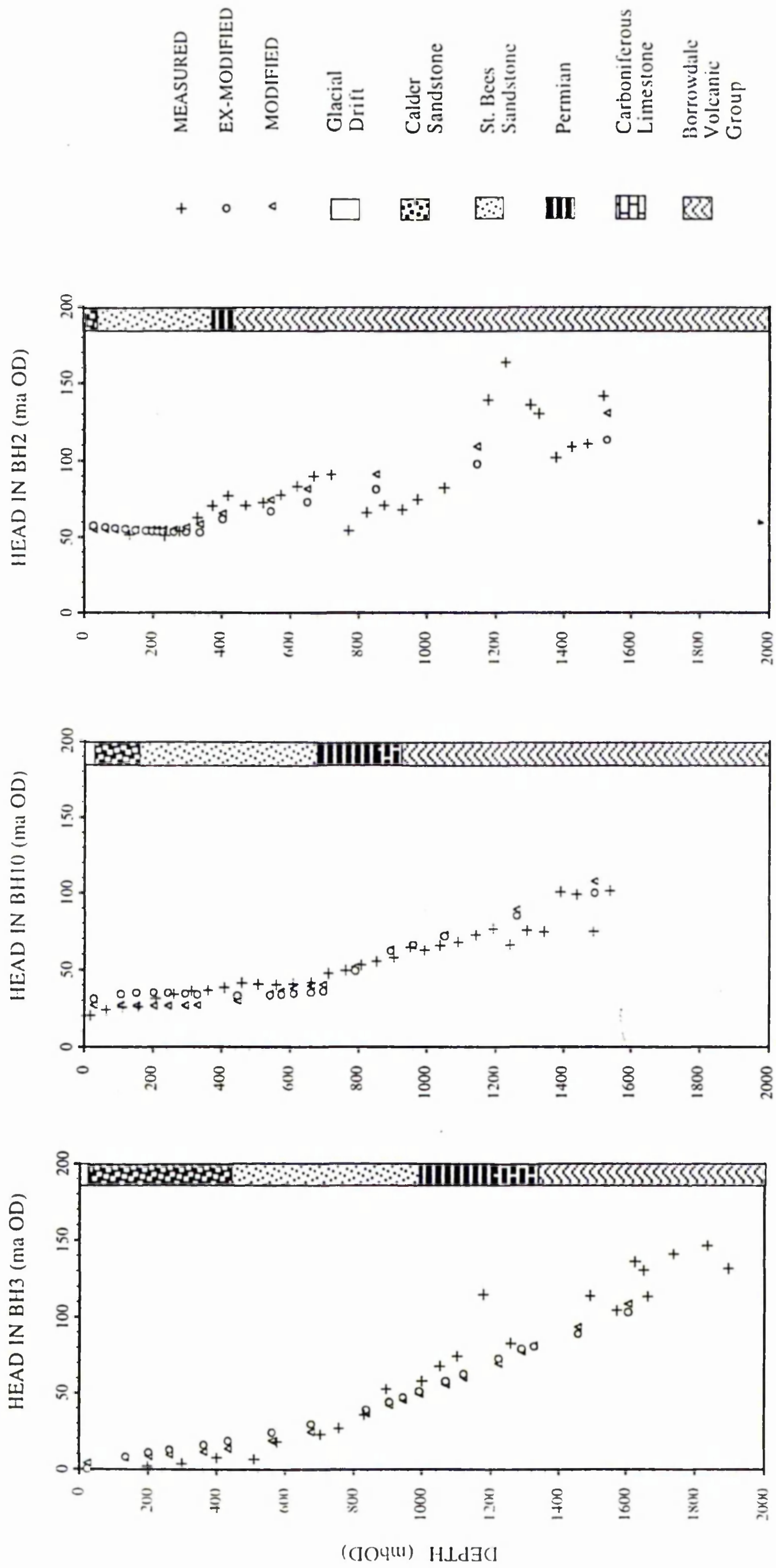


Figure 5-2 The calculated head after the modification of the mesh

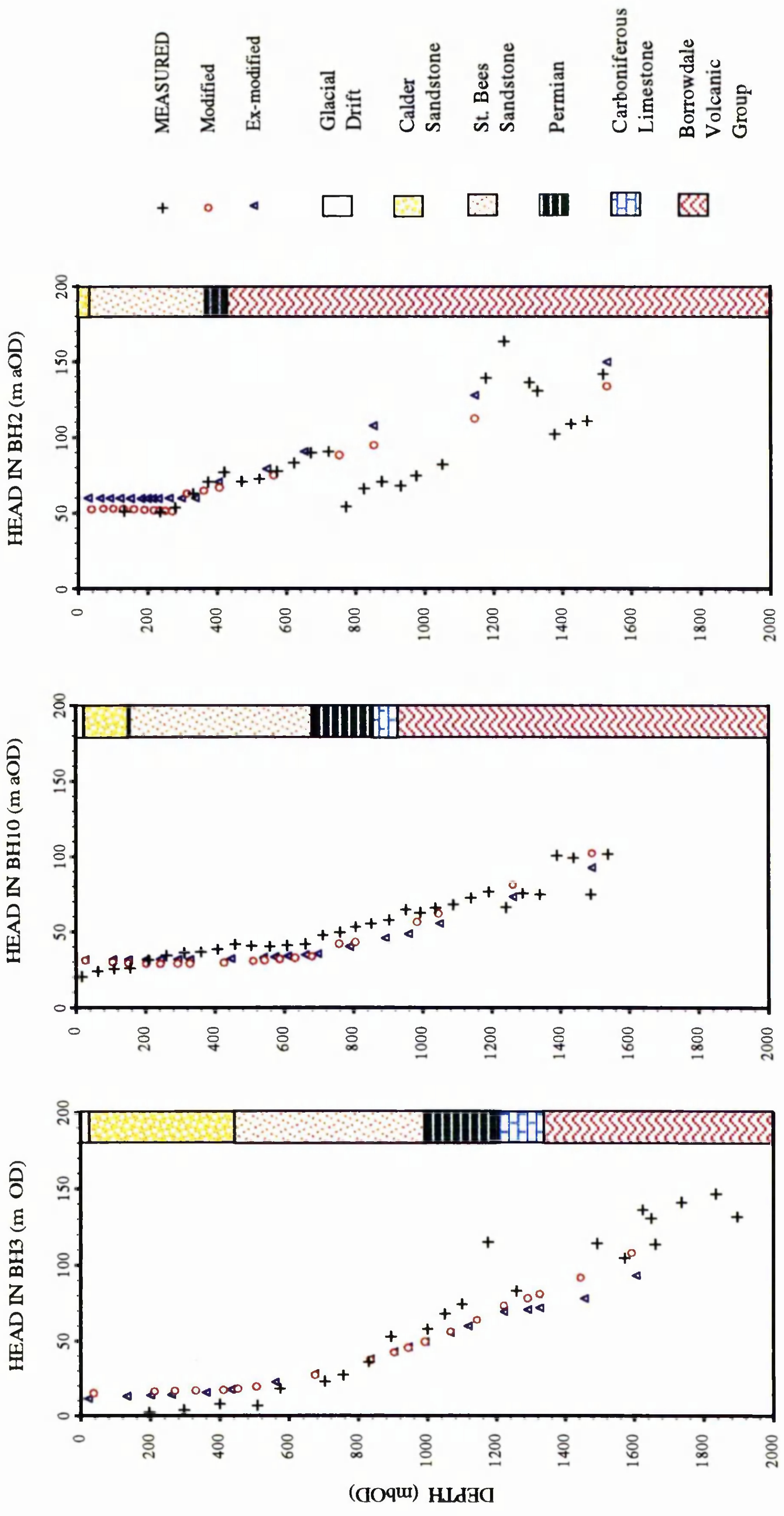


Figure 5-3 The modelled head as a result of modification of the fault

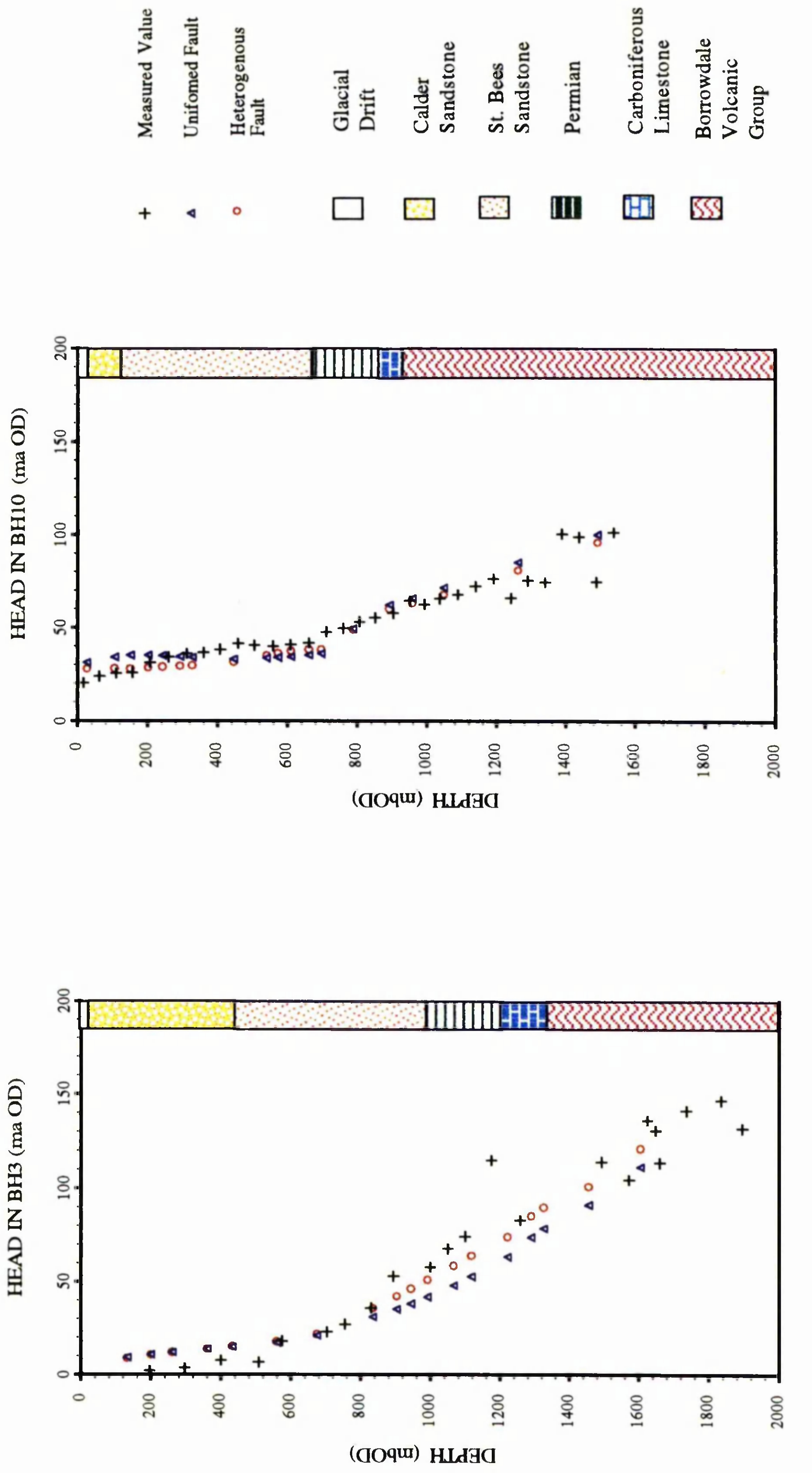


Figure 5-4 The modelled head as a result of introducing heterogeneity of the faults in the Modified Model

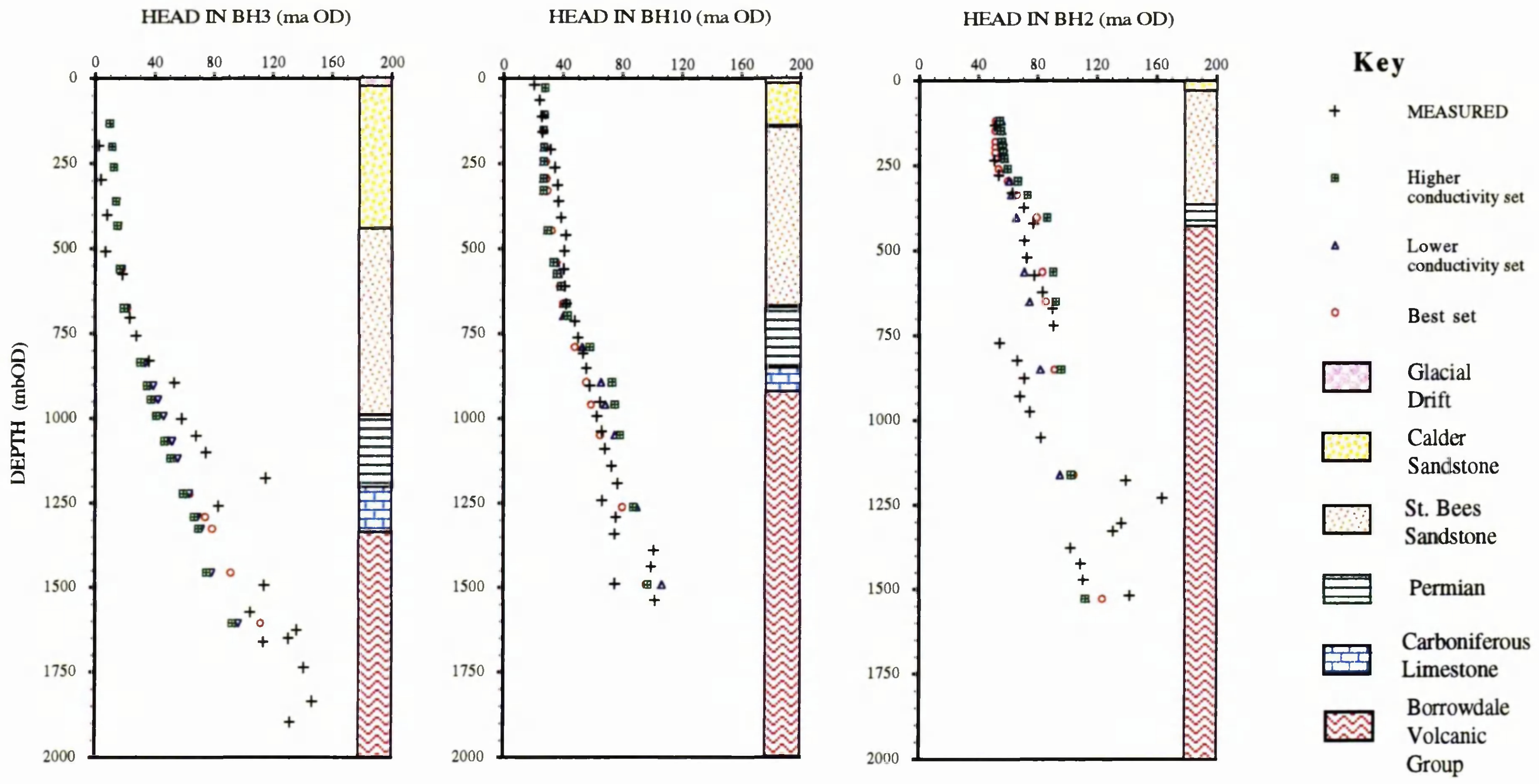


Figure 5-5 The calculated freshwater head using several suites of the parameters among which only one set fits the modified model. The other sets that fit the previous models do not fit the modified model.

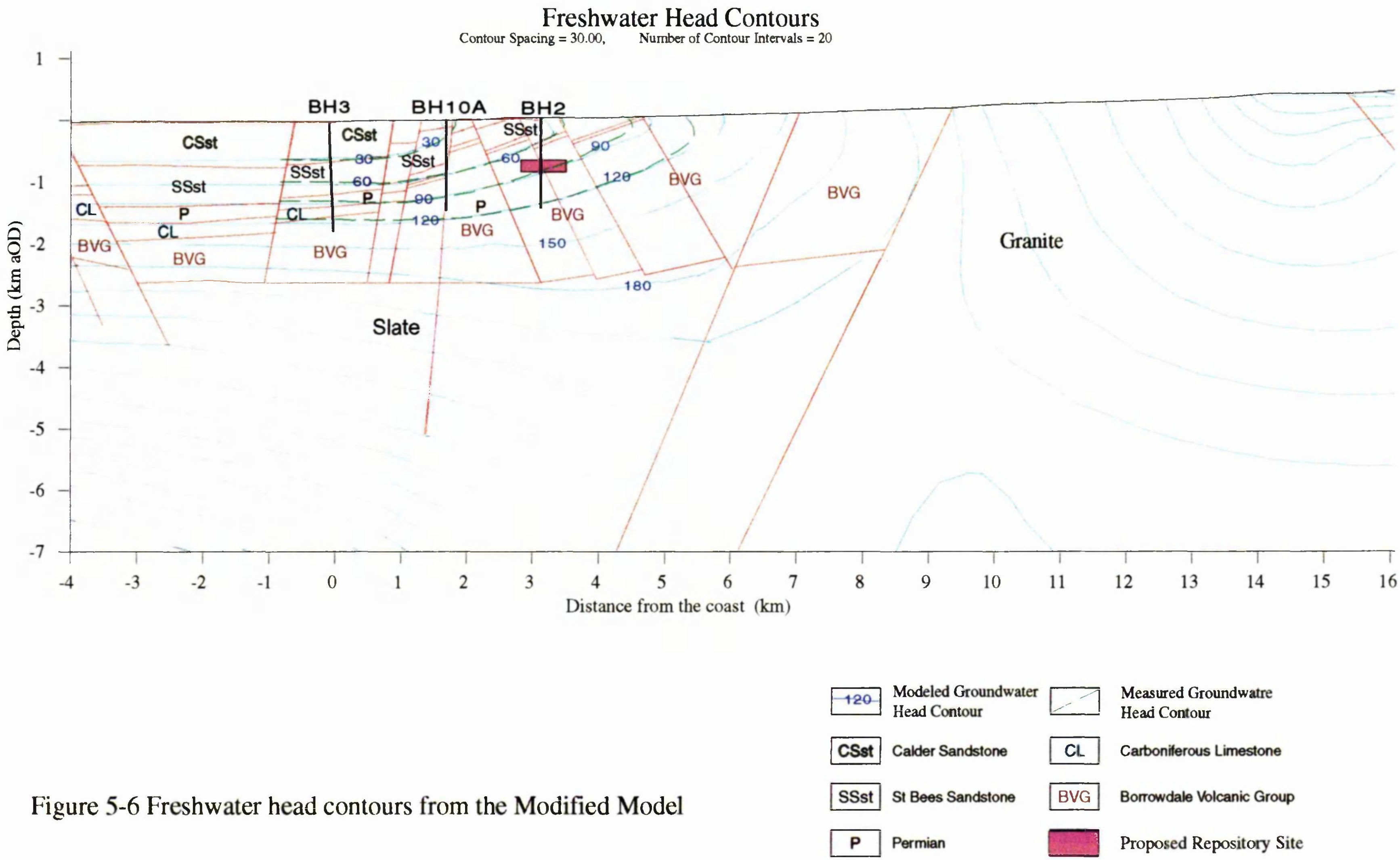


Figure 5-6 Freshwater head contours from the Modified Model

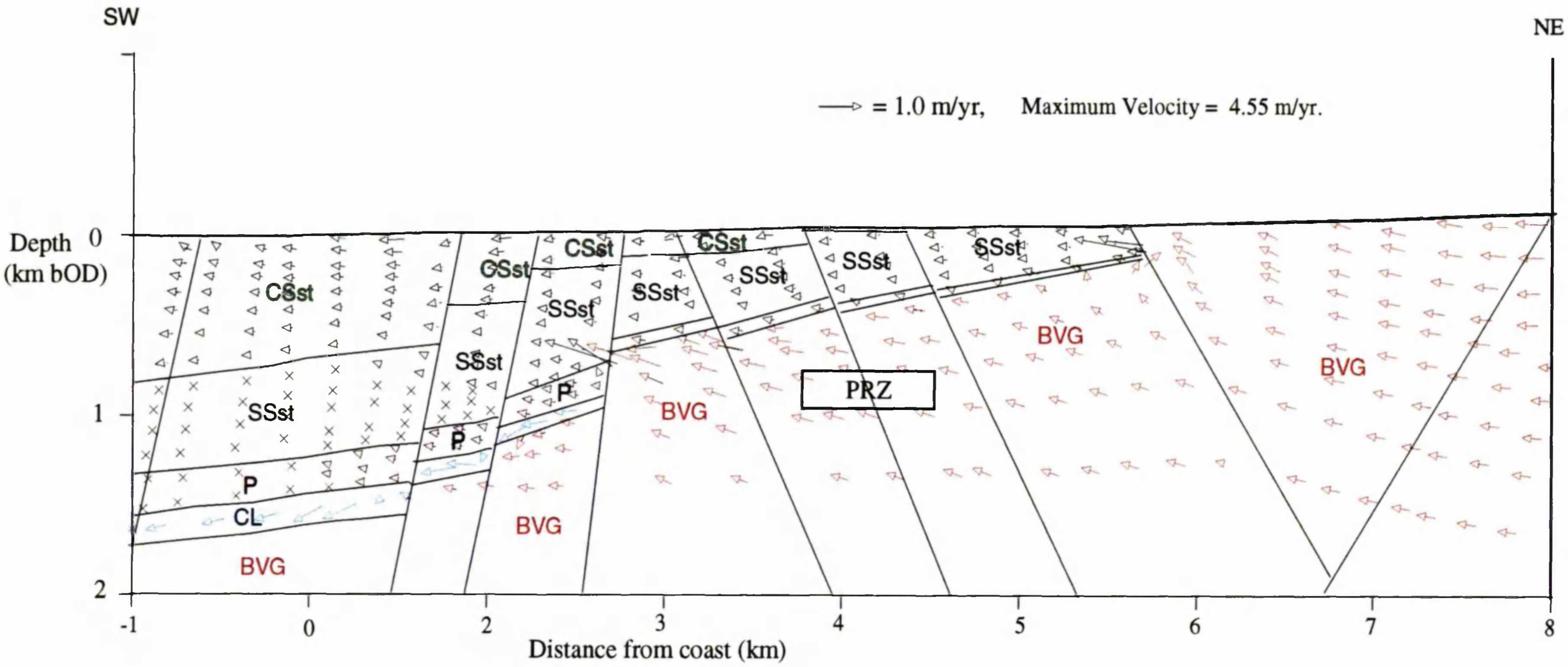


Figure 5-7 Groundwater velocity field from modified regional model along the cross section at Sellafield. The flow rate at the repository site is about 0.8 m/yr.

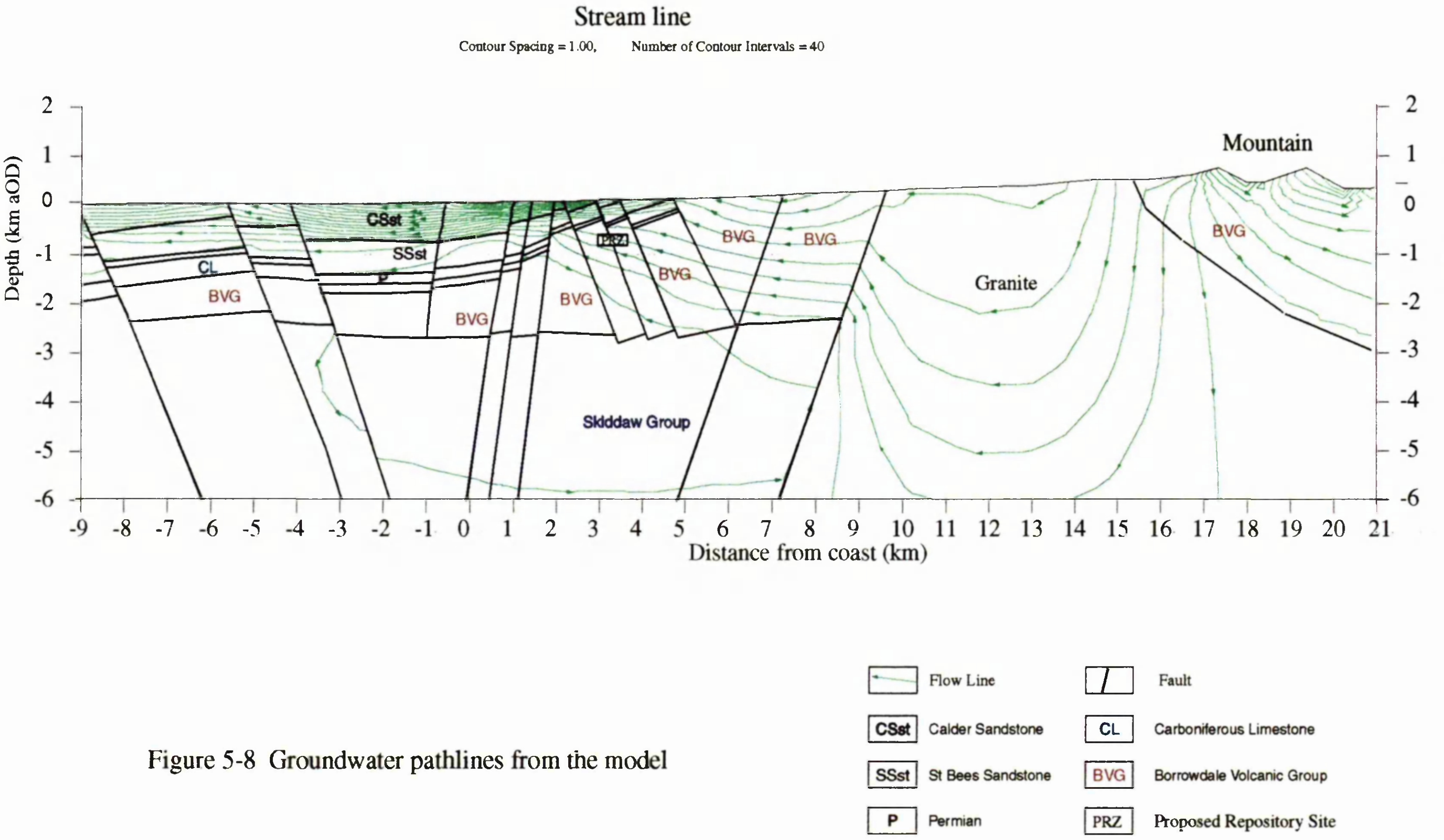
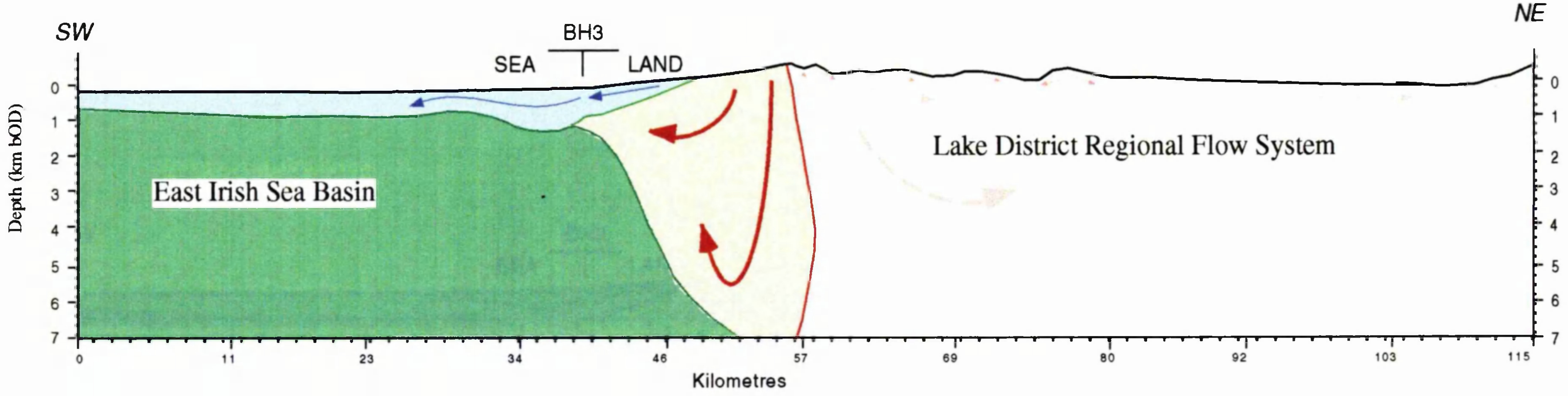


Figure 5-8 Groundwater pathlines from the model



Explanation

Figure 5-9 Regional Groundwater Flow System Regimes Division in West Cumbria

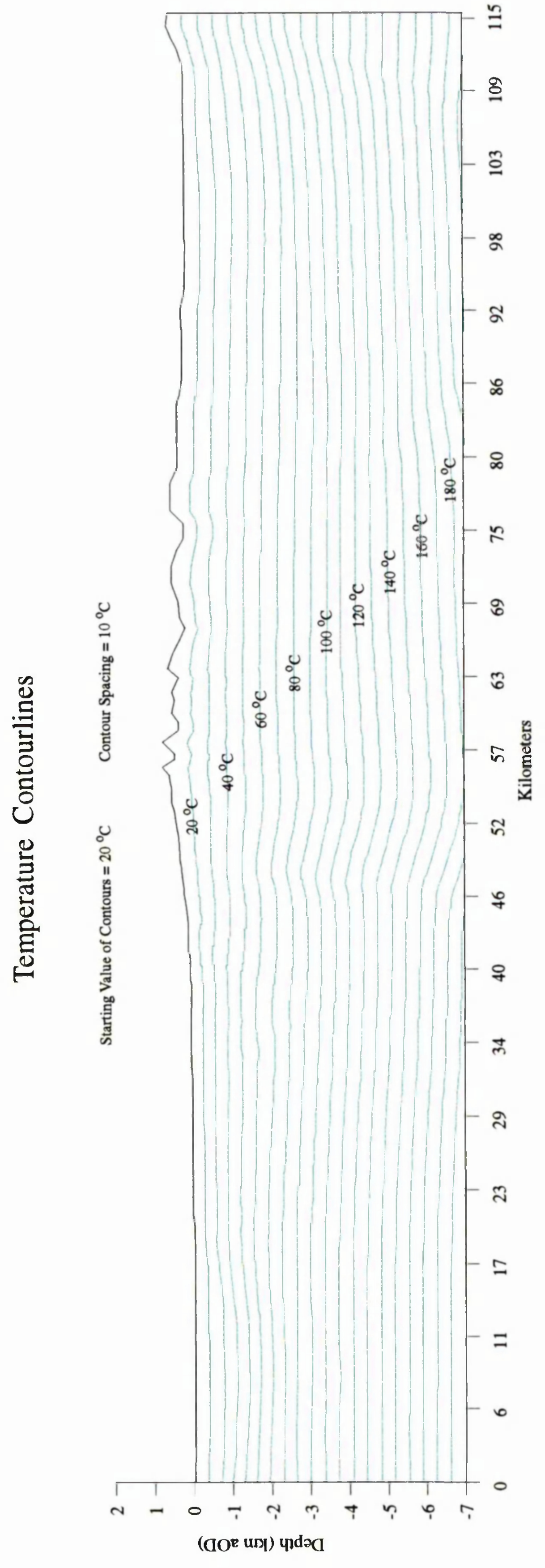


Figure 5-10 Temperature Distribution from the Modified Model

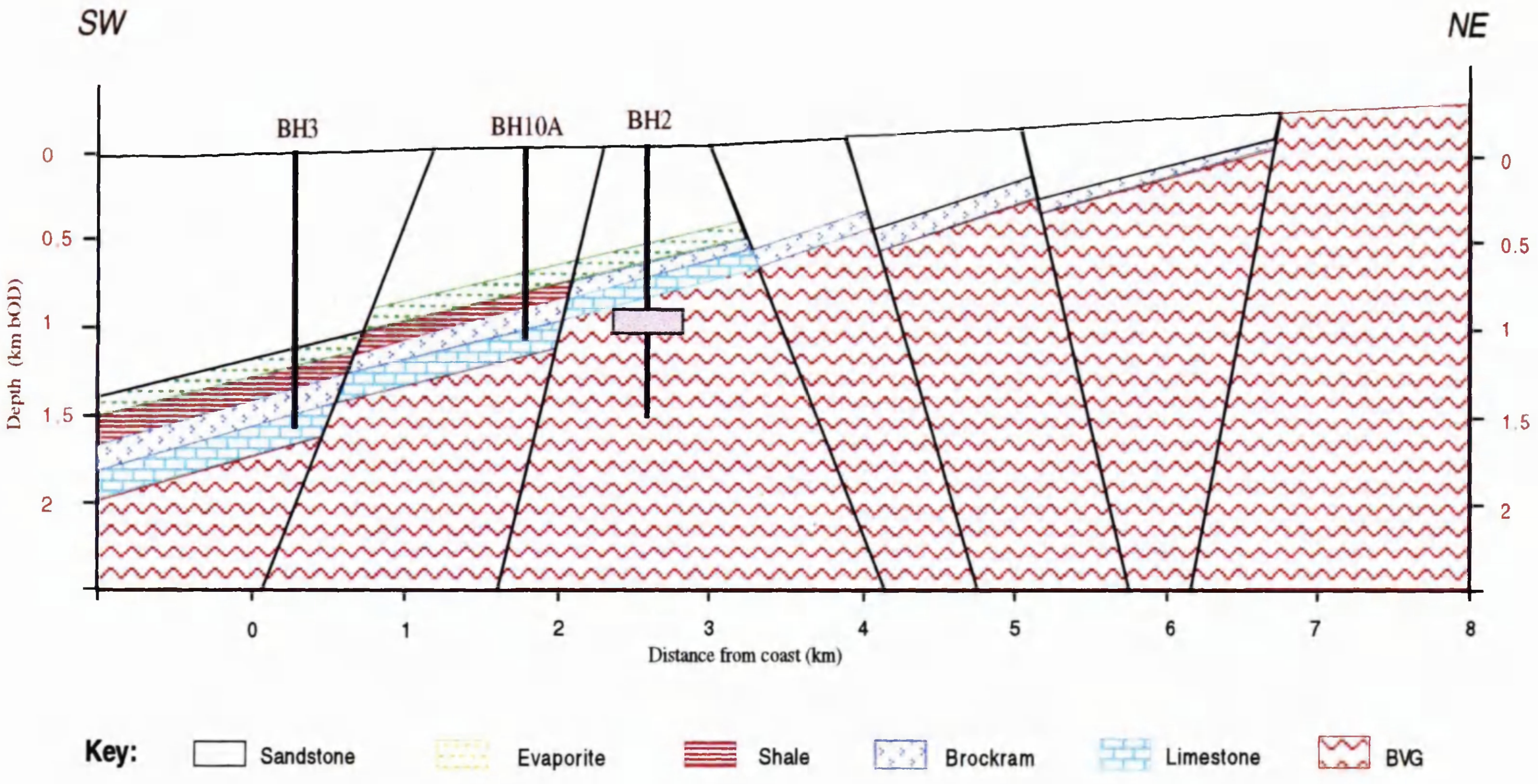


Figure 5-11 The idealised Geological Cross Section used by NIREX (NIREX, 1993)

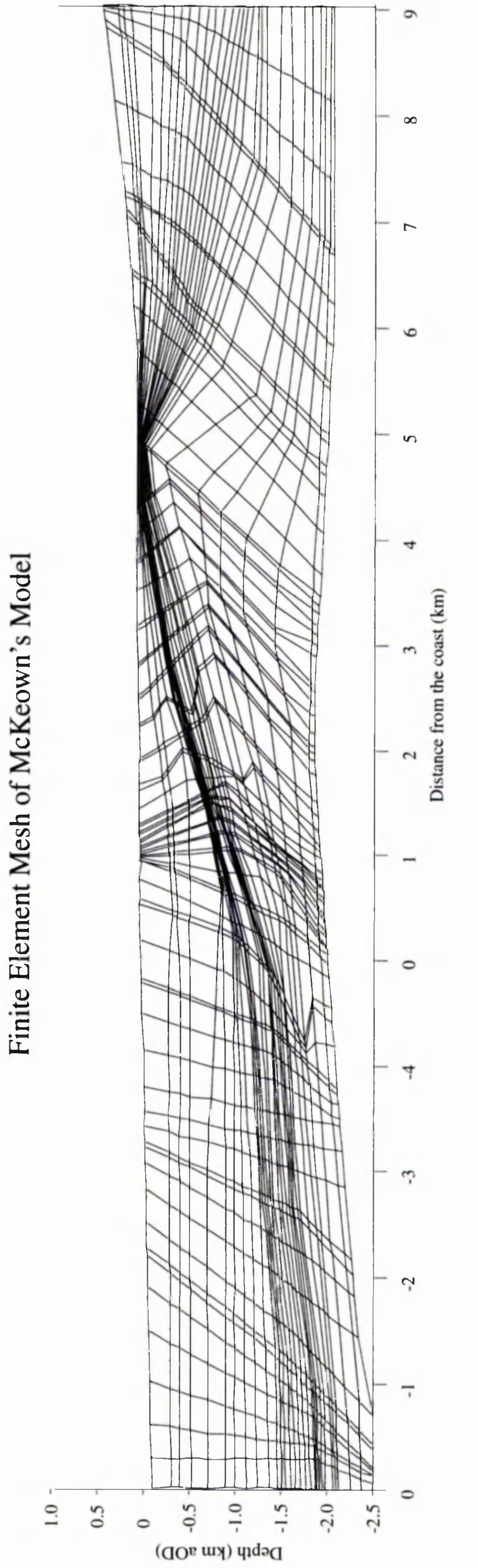


Figure 5-12 Quadrilaterals used in McKeown's Model

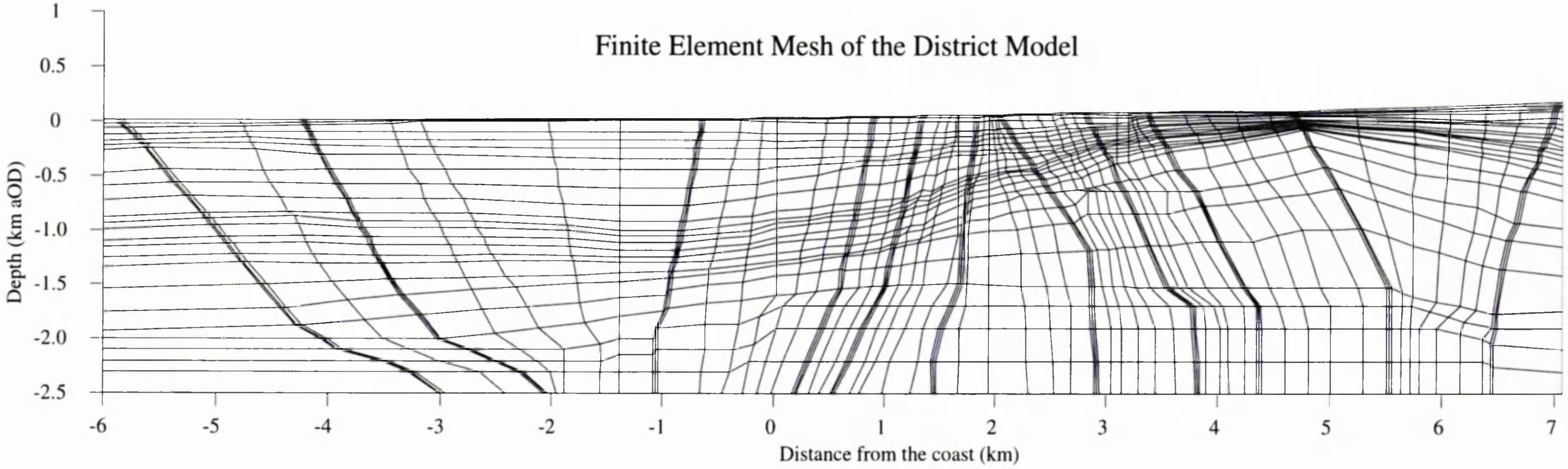


Figure 5-13 Quadrilaterals used in the District Model

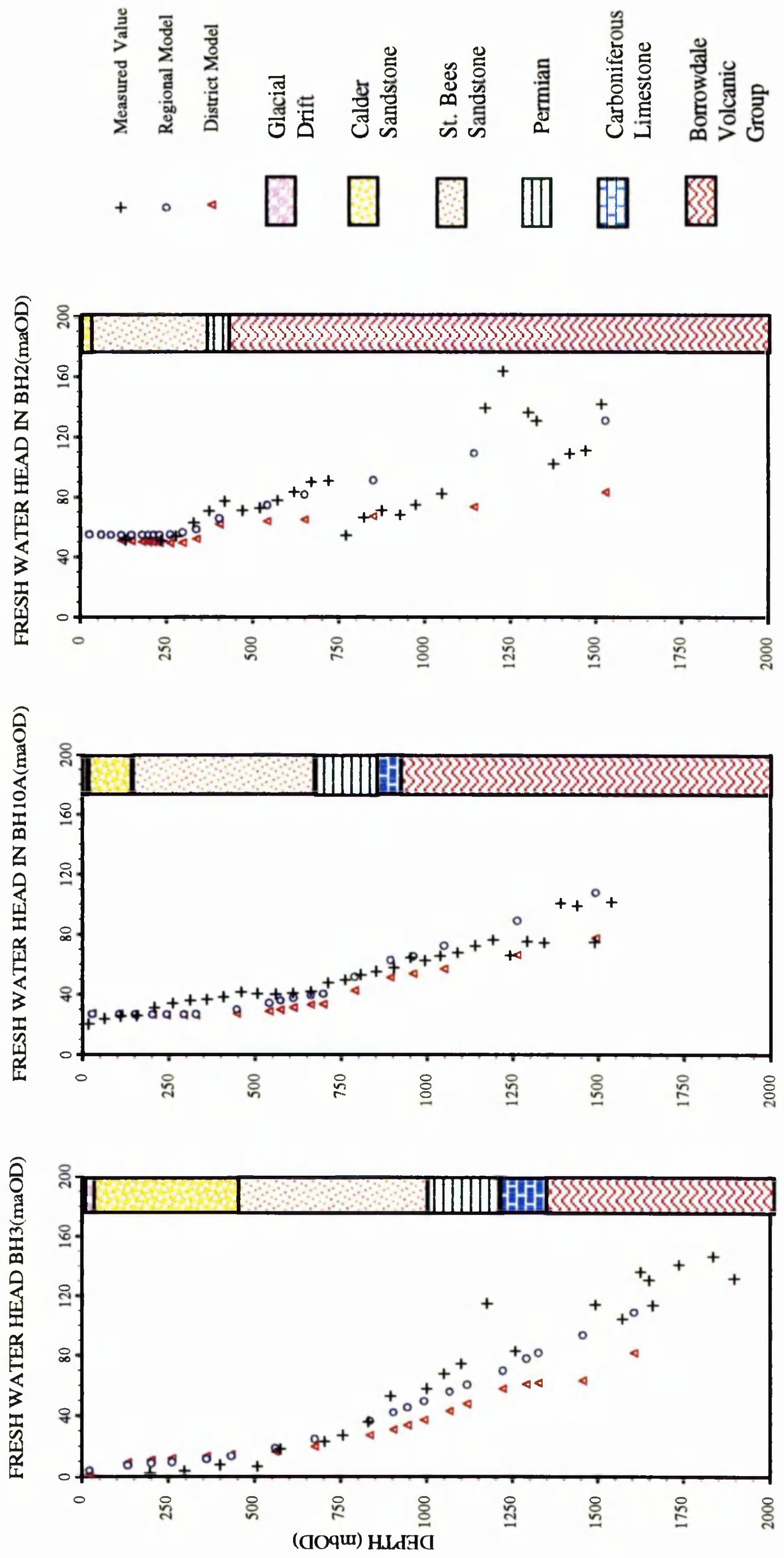


Figure 5-14 Comparison between Regional Model and District Model

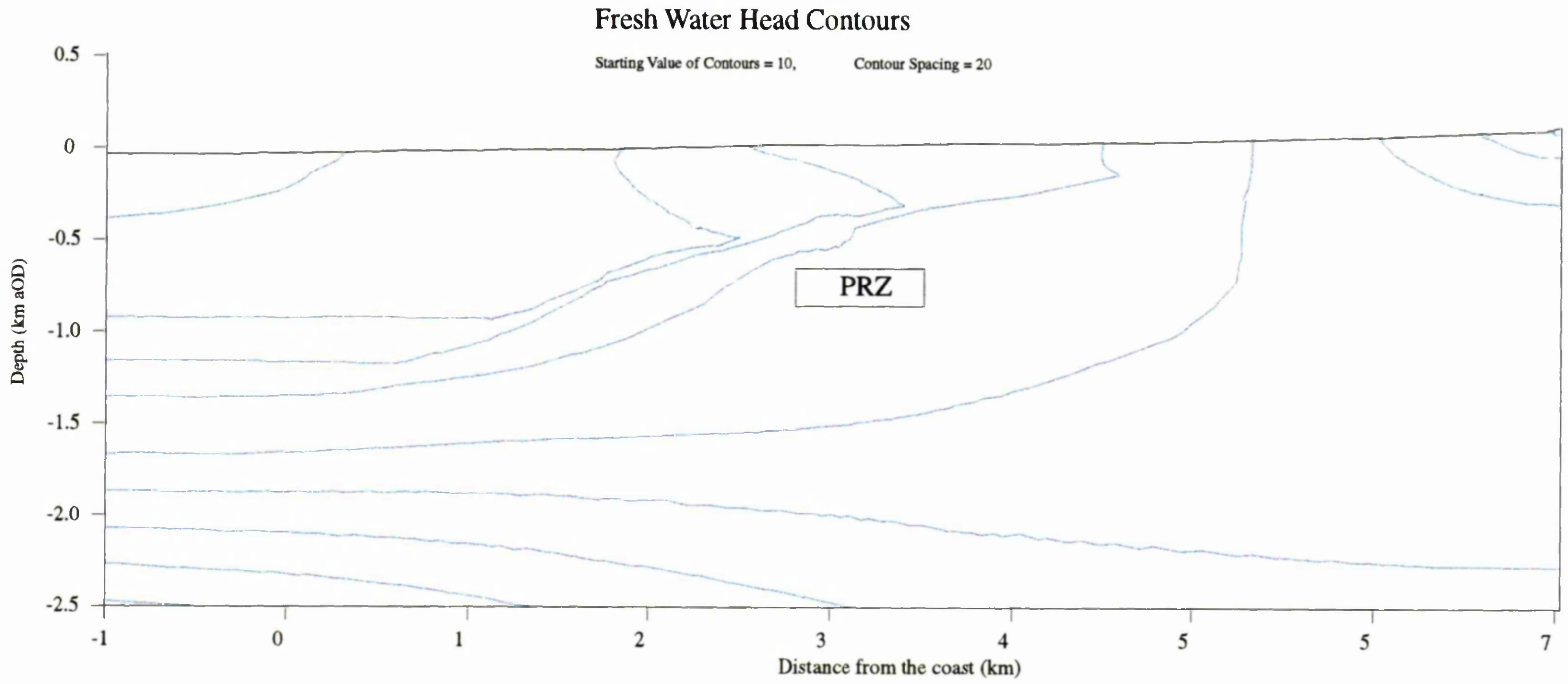


Figure 5-15 Fresh Water Contours from the District Model

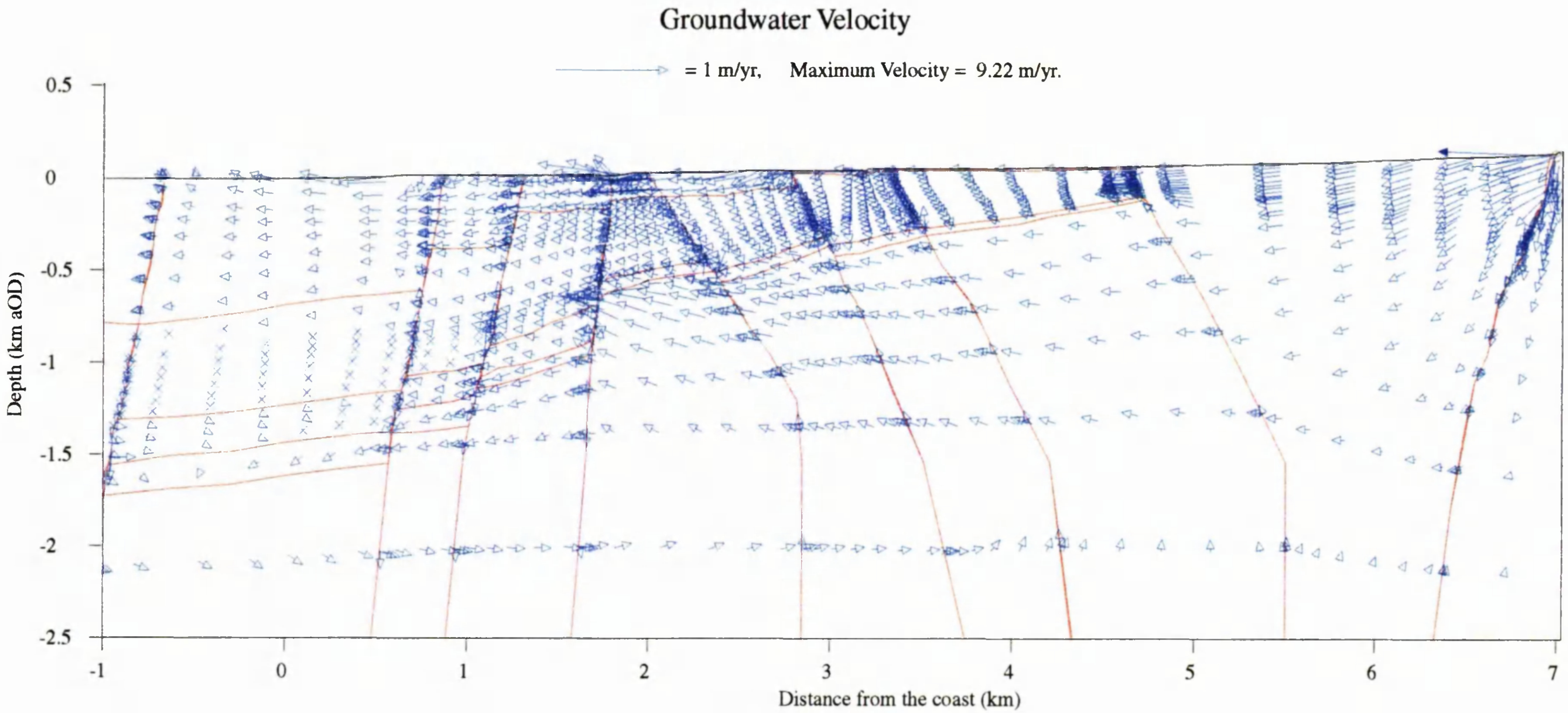


Figure 5-16 Groundwater velocity from the District Model

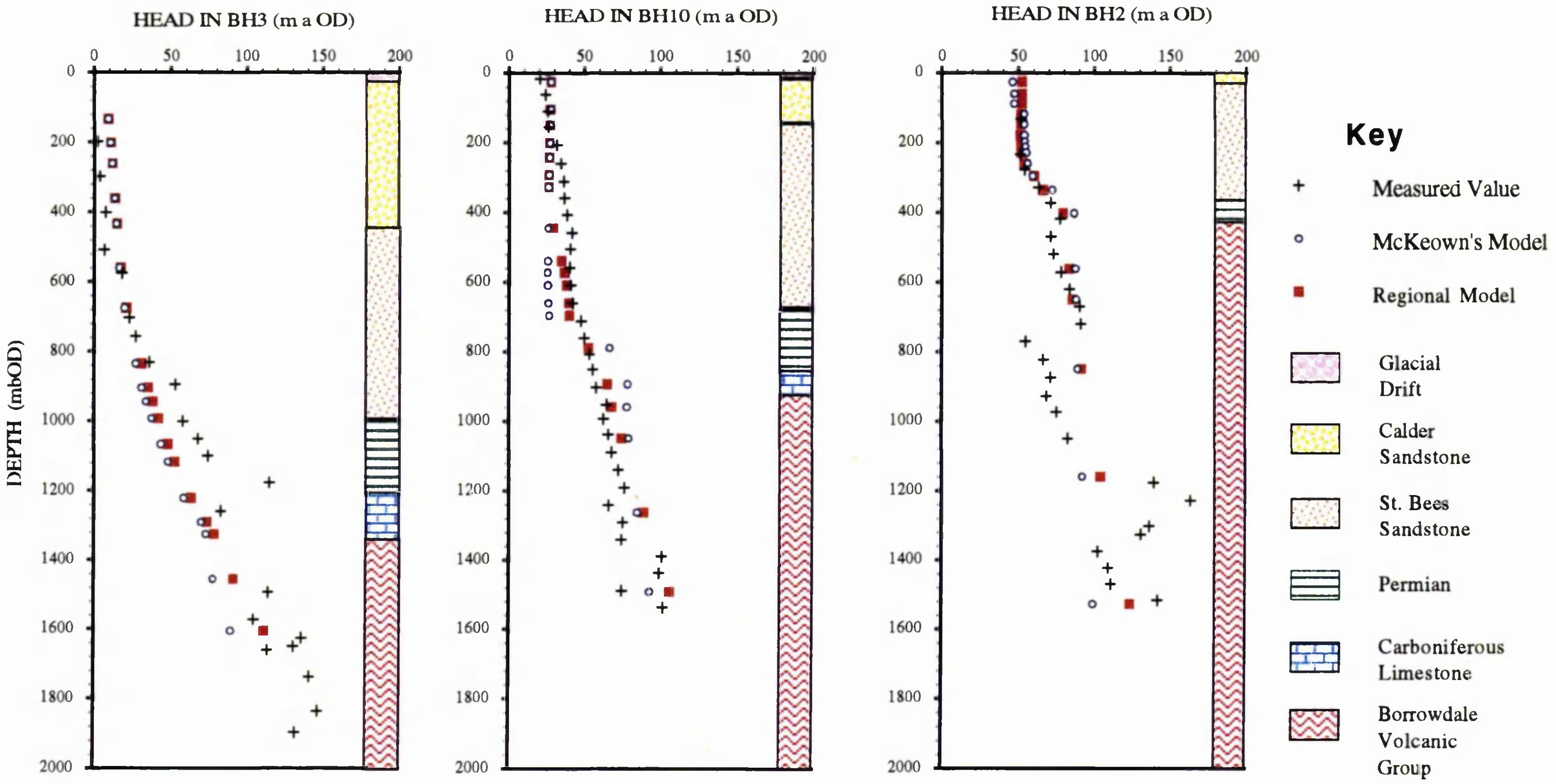


Figure 5-17 Predicted fresh water head from various models
(comparison between McKeown's model and the regional model)

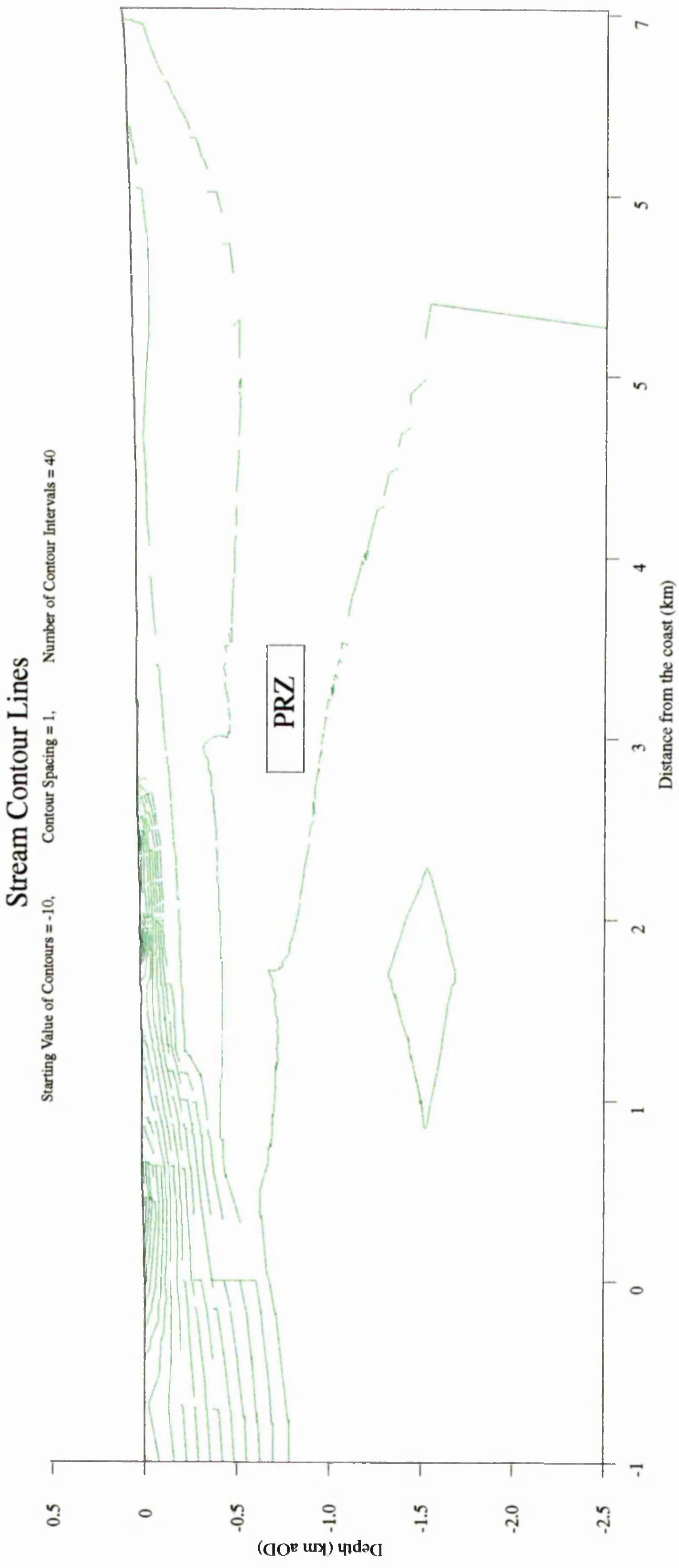


Figure 5-18 Stream Lines from the District Model

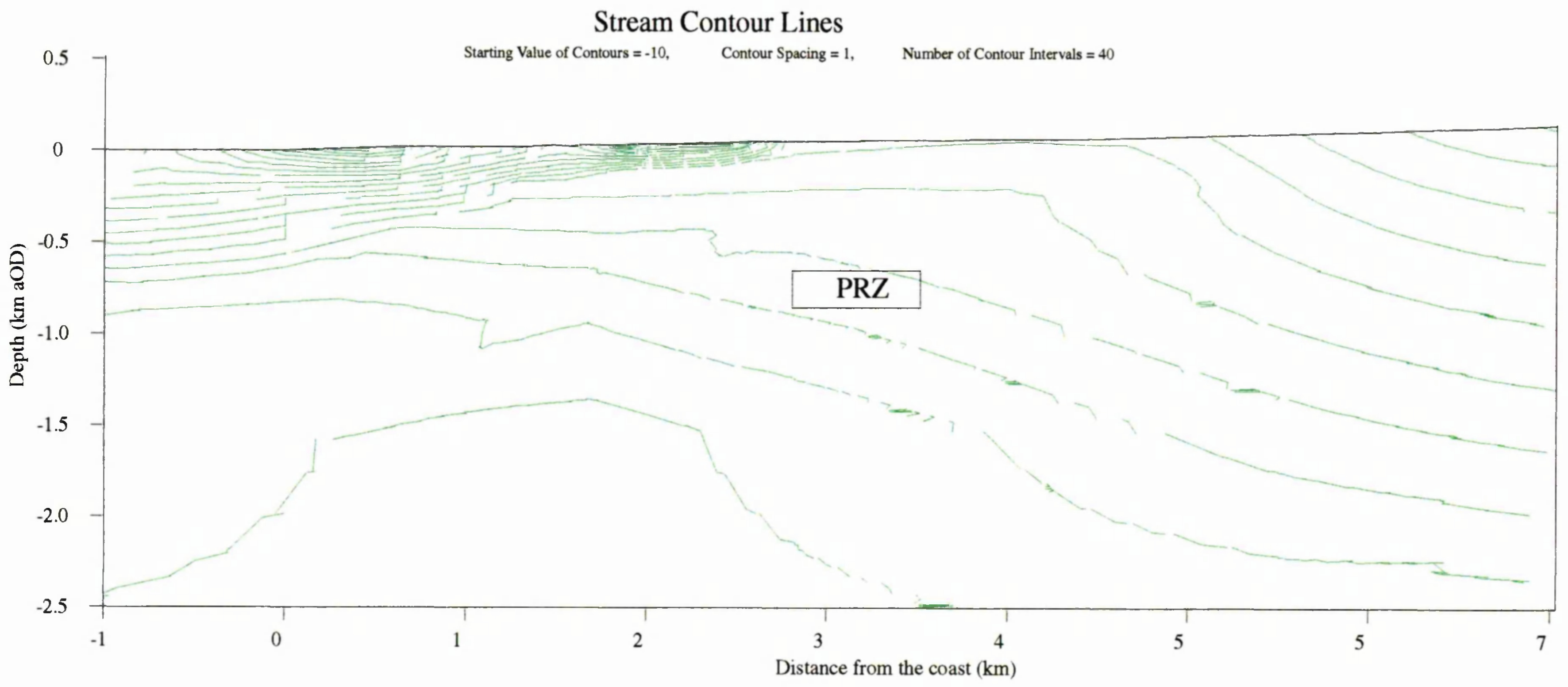


Figure 5-19 Stream Lines from the Regional Model

Chapter 6

PARTICLE TRANSPORT IN GROUND WATER

1 INTRODUCTION

The vital issue of this study is to predict the migration of radionuclides away from the repository site. Prediction should be based on well calibrated models, to provide accurate extrapolation with important sensitivities identified. In this chapter we consider the most important problems of radionuclide mass transport by groundwater through porous media. Effective management and safe disposal of radioactive waste relies on the ability to predict the migration and persistence of radionuclides underground. To simulate mass transport one must, of course, have an appropriate representation of the velocity field, which has been made fully available through the procedures described in the preceding chapters. It is still critical to choose suitable parameters to feed in to the model of mass transport in groundwater. Poor predictions, due to uncertainties in the parameters of the medium through which the nuclides are transported, result in significant safety uncertainty, and in performance, economic, and environmental costs.

Limited knowledge of the variations in fracture density, geometry and conductivity, of matrix porosities, and the complex groundwater flow field, severely restricts the ability to predict radionuclide migration at Sellafield. The previous numerical modelling of Sellafield was performed by a number of organizations working together (Heathcote *et al*, 1996). Their work emphasis was on reproducing the groundwater head at the repository site and none of their work was involved in simulating radionuclide transport. The migration of nuclear waste leakage was simulated by Haszeldine and McKeown (1999), McKeown, *et al* (1998) using OILGEN's mass transport computer program, but it was not validated. Transport parameters are very sensitive to the internal geometry of the rock medium. Consequently misestimating of the geometry may cause misleading errors in prediction of contaminant movement (Carrera, 1993).

One approach to the problem is to use hydrogeochemical data to determine effective transport parameters directly. Radionuclides which leach from a repository of nuclear waste in the volcanic rock are transported by the groundwater in a very complex fracture network. In my research the recharge of the groundwater at the repository site has been determined by means of a regional groundwater flow model. A more effective method of determining transport parameters directly is by fitting models to measured field data of groundwater age. The groundwater residence time has been measured directly from field samples in boreholes (Bath *et al*, 1996). This has involved different dating techniques ranging from ^{3}H (sensitive to ages less than 100 years); ^{14}C (age limit 40,000 years); and He content or ^{36} Cl (sensitive to ages greater than 10^6 years). Groundwaters at Sellafield in the PRZ have an average residence age between 10^4 and 10^6 years (NIREX, 1997). The groundwater age can also be determined by investigating groundwater travel times using a groundwater flow model (Toth and Sheng, 1996). In that study the travel times were estimated by interpolation between computed isochron values, and travel distances were expressed as relative lengths along flow lines passing through the reference point. However diffusion was not considered in their simulation. In my study, the migration of groundwater from recharge areas to the repository site was simulated using OILGEN's mass transport computer program, and both dynamic dispersion and molecular diffusion are involved in this study. My approach is to validate the mass transport model using data of groundwater residence age. After this, accurate prediction of radioactive waste leaching from the storage site can be made through the regional model. The objective of this modelling is to investigate the pathways of groundwater and radioactive waste movement from the mountain area through the underground disposal site and then leakage discharge through the subsurface system. It is also useful to assess the safety position by investigating the discharge pathway of groundwater, and to evaluate the return path and return time of potential radionuclide migration from the storage site. It is stressed that such investigations do not constitute a full performance or safety assessment but that discharge return time is an important contributor to overall performance.

In this chapter, the principles of mass transport and particle tracking methods are outlined. This is followed by discussion of the field measurements of groundwater age at Sellafield. Both the hydraulic parameters of the rocks and flow lines of groundwaters can be evaluated using chemical data. Then the mass transport model is validated by fitting models to data of groundwater age. With those uncertainties being fixed, finally it is possible to make predictions under those validated circumstances.

2 PARTICLE TRACKING MODEL

This transport model is based on the principle of conservation of mass. Advection and dispersion are regarded as being the major phenomena transporting radionuclides leaching from the nuclear waste repository. The flow-rate of water in the ground is calculated by Darcy's law and the transport of solute is done by the so-called advection-diffusion equation.

2.1 Governing Equations

The aim of the transport model is to simulate the migration of elements due to advection and diffusion. Derivation of the governing transport equations for radioactive solutes is presented in Huyakorn, *et al* (1983). We can approximate the solution of the advection-dispersion equation for one species in a single phase system as

$$\frac{\partial c}{\partial t} + \bar{R} = \nabla \cdot (\bar{D} \nabla c) - \bar{V} \cdot \nabla c \qquad (6\text{-}1)$$

where c is the mass concentration, $\bar{V}$ is the average linear velocity, $\bar{R}$ is defined as the heterogeneous rate of reaction, $\bar{D}$ is the dispersion coefficient. The chemical reactions are most commonly considered as in equilibrium radioactive decay. For the linear isotherms the retardation factor R_d is defined as:

$$R_d = 1 + \frac{(1-n)\rho_s k_d}{n}$$

where n is the porosity, k_d is called the distribution coefficient and (6-1) can be rewritten as:

$$R_d \frac{\partial c}{\partial t} = \nabla \cdot (\bar{D} \nabla c) - (\bar{V} / n) \cdot \nabla c \qquad (6\text{-}2)$$

The dispersion tensor is expressed as (Bear, 1972):

$$D_{ij} = a_T V \delta_{ij} + (a_L - a_T) V_i V_j / V + D_d \tau \delta_{ij} \qquad (6\text{-}3)$$

where a_L is the longitudinal dispersivity and a_T is the vertical dispersivity, D_d is the coefficient of molecular diffusion, τ is the tortuosity.

The mean value of the water velocity, as determined by Darcy's Law, results in advection with a bulk displacement of the element. The additional flux resulting from the fluctuating velocity in the vicinity causes the spreading or dispersion. In low permeability rocks, the transport from molecular diffusion is not negligible and it could even be dominant in some cases. The advection and dispersion relies on the local velocity vector, so the migration of chemical elements strongly depends on the ground water flow field. Chemical reactions and effects of adsorption/desorption are ignored at this stage of modelling.

2.2 Random walk method

The advection-dispersion transport equation is more difficult to solve numerically than the flow equation. Traditionally, the solution of the advection and dispersion equation for transport uses finite difference and finite element methods (Kitanidis, 1994). These yield numerical dispersion, resulting from the conflict inherent in the solution of an equation that simultaneously contains parabolic terms (dispersion) and hyperbolic terms (advection). The discrete particle tracking (also known as random walk) method is an alternative which solves both advection and dispersion by a hyperbolic type method (Prickett *et al.*, 1981). The mass transport program uses a 'particle tracking' technique to simulate the physical behaviour of mass transport in groundwater flow. The basic idea is to approximate the transport of the mass of solute by a cloud of discrete particles. Each particle is displaced in successive steps to represent advective and dispersive processes in the groundwater flow field. Advection occurs naturally according to the average path and velocity of a particle that is moved passively in a groundwater flow field. Dispersion is the process simulated by a random walk movement following a normal distribution by which the movement of any individual particle varies from the average advective path. Concentrations can be calculated at a specified time by evaluating the number of particles within a specified search volume, taking into account the mass of each particle at that time.

The particular advantage of the random walk method, is that it performs well for large Peclet numbers (Kitanidis, 1994). The local grid Peclet number is the ratio of the typical advective velocity times the grid size (length) divided by the dispersion coefficient (Furbish, 1997). The element size should be selected so that $\Delta l \leq 10D/V$, where Δl is the characteristic length of the element, and the time-step should be selected such that $\Delta t \leq \Delta l/V$. In large-scale modelling this number is large, thus the transport equation behaves as a hyperbolic partial differential equation for which solutions from direct application of finite difference or finite element formulations are affected by numerical dispersion or oscillations (Huyakorn and Pinder, 1983). The other advantages of the random walk method are that it conserves mass, even if the flow field is not computed with high precision, and may not require the solution of large systems of equations.

The disadvantage of the random walk method is that the determined concentration function is not smooth (Sun, 1989). To increase the smoothness a large amount of CPU time is needed. However this method is well suited for this study because even a trace amount of the radioactive waste is vital in the assessment of potential migration away from the disposal site. In predictions of radioactive waste migration, what we want to understand is the first arrival of the nuclides. To this end, a fully implemented particle tracking method is the most effective way to help us investigate it.

2.2.1 *Numerical procedure*

Like other numerical methods, the random walk method is also performed on the discretised mesh. The particle tracking method is different from the previous numerical procedure. It does not solve the mass transport equations directly but simulates the spread of mass dissolved in water. A particle can be seen as a very small plume, assumed size of zero. For each time step, every particle is separately advected and dispersed. The advection occurs coincidentally with the local flow velocity, and the dispersion is expressed as a random movement that is divided into a component coincident with the flow vector and a component transverse to the flow path. The standard derivation and the movement of one particle in a two dimensional problem of dispersion is:

$$x(t+\Delta t) = x(t) + V_x \Delta t + (2\,\alpha_L V_x \Delta t)^{1/2}\,\xi + (2\,\alpha_T V_y \Delta t)^{1/2}\,\xi \qquad (6\text{-}4)$$

$$y(t+\Delta t) = y(t) + V_y \Delta t + (2\,\alpha_T V_y \Delta t)^{1/2}\,\xi + (2\,\alpha_L V_x \Delta t)^{1/2}\,\xi \qquad (6\text{-}5)$$

where t is the time, x, y is the horizontal and vertical distance respectively, V_X, V_y is the horizontal and vertical flow velocity respectively, a_L is the longitudinal dispersivity and a_T is the vertical dispersivity, ξ is an independent normally distributed random variable with average 0 and standard deviation 1. The oscillations due to the stochastic aspects of the method can be reduced by increasing the number of the particles. When a sufficiently large number of particles are applied to the above process the spatial density of these particles yields solute concentrations with an acceptable precision. The total mass in every cell can be known by summing the mass given to the particles present, and the spatial concentrations can be obtained by superimposing a discretised mesh over the particle distribution. Although the velocities are space dependent in this study area, equation (6-4) and (6-5) consist of displacing the particles along streamlines for longitudinal and for transverse dispersion, thus directly accounting for the local variations in velocity.

2.2.2 *Boundary conditions*

All the bottom, and the two vertical lateral boundaries are impermeable to mass transport. Chemical elements are free to leave or enter the flow domain along the water table.

2.2.3 *Solution procedure*

The flow chart of the mass transport model is presented in Figure 6-1. When the flow field is determined through the groundwater flow model, the advection is calculated and the displacement of advection is obtained for each time step. By generating the random variable and using the equations (6-4) and (6-5), the total movement of a particle can be obtained. After each movement the new position of the particle is specified and the movement across the boundary of the element must be justified according to the boundary conditions (Garven and Freeze, 1984). Concentrations of the chemical elements can be known just by counting the number of the particles in the element and the mass given to every particle. This calculation is repeated in accumulating time steps, until the time reaches the pre-set period. It should be noted that the time step should be small enough so that the particle movement is within the limited distance of one single grid at each time step.

The transport of particles is restricted by the boundary conditions, the particle must be checked during each time step in order that the mass is not transported across a no-flow boundary during its movement.

The grids and mesh used in this model are based on the mesh used in the groundwater flow model. In order to increase the precision of the flow field, the mesh within the Sellafield site was intensified to reduce the Peclet Number (Figure 6-2). This mesh also deletes the irrelevant parts from the eastern natural no-flow boundary.

3 ORIGINS OF GROUNDWATER AT SELLAFIELD

3.1 Introduction

The groundwater is formed or originated from precipitation in the recharge area, then flows towards the discharge area. Recharge is assumed to be perfect and continuous, due to the high rainfall of the recharge area (>3000 mm/yr). During its movement, there are always chemical reactions in groundwaters, the medium through which the water flows, and chemicals in the water. These reactions can be known by analyzing the components and their changes in the water. Some components, such as isotope data, can be used to date groundwater age. The older groundwater is, the more complex and mixed it will be and more likely subject to a complex evolution that might affect the reliability of the hydrochemical or isotopic information. Knowledge of solute residence time and groundwater age is important, in that it helps in understanding the rate of processes within, and time of recharge into the groundwater system.

There is a variety of natural isotope systems in groundwater which can be applied to groundwater age, such as tritium (half-life 12.3 yr), carbon-14 (half-life 5730 yr) for short period age, chlorine-36 (half-life 301,000 yr), uranium-thorium natural series (half-life>10^6 yr) for long time aged water. Stable oxygen and hydrogen isotopes are qualitative inferences of glacial or non-glacial climate and can also be used to indicate appropriate recharging time.

3.2 Hydrochemical and Isotope data at Sellafield

3.2.1 *Chemical compositions*

During the appraisal of Sellafield, many groundwater samples were collected from boreholes. The details are reported by NIREX (NIREX, 1993). The basic hydrochemical data obtained from Borehole 2 and Borehole 3 water sample analysis are presented in Table 6.1 and Table 6.2. The hydrochemical features of groundwater at Sellafield can be divided into Na-Cl dominated saline waters in the BVG at depth and shallow Ca-Na-HCO_3 dominated dilute waters in the Sandstone Group. The shallow groundwater has features of the precipitation in this area. Additionally there seems to be mixing with a source of deep saline water that could contribute to increased chloride. Based on NIREX (NIREX, 1993), the deep groundwater hydrochemical parameters vary from Borehole 3 near the coastline to Borehole 2 at the proposed disposal site.

The variation of salinity was observed and calculated from the total dissolved solid values for the groundwater samples or on the basis of electrical conductivity data (NIREX, 1993). The Br:Cl ratio in the saline groundwaters in Borehole 2 is higher than in Borehole 3 suggesting that there might be two sources of salinity (Figure 6-3). The differences between the two sources can also be shown in the plot of Na versus Br (Figure 6-4), a higher gradient of brines in Borehole 3 than the saline waters in Borehole 2, the saline groundwaters from Borehole 10 plot between them. All the differences in groundwater chemical components reveal that their origins are different. The basinal component is dominant in Borehole 3 at the coastline. The inland component is dominant in Borehole 2. The components are mixed in Borehole 10A standing in the middle.

3.2.2 *Isotopic Compositions and Groundwater Age*

Based on the NIREX report (NIREX, 1995), a few isotopic data have been analysed to constrain recharge timing of the groundwater at Sellafield. These are: stable isotope ratios for oxygen and hydrogen ($\delta\,^{2}H$ and $\delta\,^{18}O$); noble gas recharge temperatures; tritium levels; carbon-14 results; chlorine-36 ratios; helium levels. All these test results can be summarised as follows:

The stable isotopes ($\delta\,^{2}H$ and $\delta\,^{18}O$) for groundwater samples in the basement rocks of the repository site have a meteoric signature, the samples taken from Borehole 2 have a meteoric signature that is lighter than that of present day rainfall (Figure 6-7). The lower BH2 samples have a distinct isotopic signature which is lighter (i.e. lower $\delta\,^{18}O$) than the groundwater in the overlying sediments, this indicates that the deeper groundwaters have an origin distinct from the shallow waters (Figure 6-6). Conversely, a trend of increasing $\delta\,^{18}O$ from -7‰ to -5 ‰ with increasing depth is seen in Borehole 3. Because isotopic fractionation effects are increasingly pronounced at lower temperatures, the lighter isotopic signature in Borehole 2 water samples may indicate that the temperature of this recharge groundwater was colder than that of groundwater in Borehole 3. In addition, it is also possible that groundwater in deep BH 2 originated from higher altitude precipitation because the isotopic composition of meteoric water becomes lighter with increasing altitude. The correlation between $\delta\,^{18}O$ and Cl at depth of BH 3 is typical of basinal brines and indicative of very long residence times in the basin (NIREX, 1995).

Stable isotopic signatures in the basin brines of BH 3 are heavier than those elsewhere in the region (NIREX, 1995), which might imply recharge prior to the last glacial epoch. In Borehole 10A and within the sandstone to the west of the site on the base of the coastal plain regime, the isotopic values are also lighter and these indicate an older and cooler recharge than current meteoric water.

The recharge temperatures can also be estimated from inert gas abundance. This is because the different noble gases are chemically inert, but have different solubilities controlled by temperature. The inert gas data of recent groundwaters indicate recharge temperatures around 10°C (NIREX, 1995). Noble gas abundances also indicate that recharge conditions for groundwaters in the BVG of BH 2 close to the PRZ were colder than those in the sandstones in BH3 (Figure 6-7). Both stable isotope composition and inert gas contents depend on climatic conditions at the time of recharge, and all these indicate that the recharge of basement rocks in the PRZ was under colder climatic conditions before the last glacial period ended 10,000 years ago.

The interpretation of data on carbon-14, helium-4 and the ratio of chlorine-36 to chloride, has the same conclusion. Measurements of ^{14}C had very low detectable levels of modern carbon, so that it was concluded that this could be attributable to contamination (NIREX, 1993). So the absence of ^{14}C suggests that the groundwater is in excess of 30,000 years old. The $^{36}Cl/Cl$ signature of groundwater in the basement rocks of the Potential Repository Zone ranges from 22 to 28×10^{15}, to reach this equilibrium most of the chloride in the groundwater in the BVG must have been present for around five half-lives (1.5 Ma). All these data suggest that the age of groundwater in the BVG of the PRZ is between 30,000 and 1,500,000 years (NIREX, 1995).

3.3 Modelling groundwater travel (residence) time

The groundwater residence time can also be determined by investigating groundwater travel time using groundwater flow models and mass transport models. The travel time can be estimated using a flow model simply by interpolation between computed isochron values. Travel distances are expressed as relative lengths along flow lines passing through the reference point (Toth, 1996). This method might be suited to low dispersion flow systems when the movement of water is dominated by advection. However, in low permeability rocks molecular diffusion could not be neglected, dispersion and diffusion must also be accounted for during long time and long distance migration. In this study, the particle tracking method is used and proved to be a good way to investigate the regional groundwater travel times in these low permeability rocks.

To estimate the groundwater age, or residence time, the exact recharge area or particle releasing position and the flow line must be known. The groundwater flow route can be obtained by solving the stream function equation (3-3), as was shown in Chapter 3. From the stream line we can roughly identify the possible recharge location from which the ground water might travel to the location we are interested in. Because there are dispersion and diffusion effects, the real location of the recharge had to be iteratively corrected after trying different releasing locations. The relevant recharge area is that from which particles can be released to flow towards the repository zone. By using such a flow path, the residence age of the groundwater can be simulated. The difference between the prediction from flow lines and that from advection and dispersion methods was also investigated in this study. Ultimately the parameters of rock properties used in the model can be calibrated to this measured residence age.

3.3.1 *Regional groundwater flow characterization*

The spatial and temporal distribution of flow, the fluid dynamic properties of flow and the natural manifestations of gravity-induced regional flow have been extensively studied in former chapters. Therefore, in this section the only characterizations reviewed are those that are directly relevant to the predictions of nuclear waste disposal at Sellafield.

As it was discussed before, the groundwater flow at Sellafield is driven by gravity. Groundwater flows downward from topographically high regions. Based on groundwater flux and its route, the groundwater flow system can be divided into: a Shallow Flow Region that has large flux, an Inland Flow Region with smaller flux and an Irish Sea Basin Region which has little flux (Figure 6-8). Emphasis is put on the Shallow Flow Region and the Inland Flow Region because they are directly relevant to the disposal site.

The most striking point is that the flow regime identified from groundwater flow features via the groundwater flow models, agrees well with the water regimes identified from hydrogeochemical data (Figure 2-5). The detailed groundwater flow system division is illustrated in Figure (6-8) in which it can seen that the groundwater flow in the BVG at the repository site is dominated by the Inland Flow system (saline water) that has a moderate flow rate and flux. In contrast, the groundwater flow at depth in BH3 is the basinal flow system which has little flux at very low flow rate (brine water). This is consistent with the chemical analysis results from deep borehole groundwaters.

3.3.2 *Groundwater residence time division*

Generally the residence time of groundwater depends on the length of its travel route and the velocity of the flow. So it is reasonable that the groundwater residence at Sellafield can also be divided into a Short Residence Region and a Long Residence Region coinciding with the Shallow Flow Regime and Inland Flow Regime. This is because the flow path in the Shallow Flow Regime is much shorter and the flow rate is relatively higher than that in the Inland Flow Regime.

Based on stream lines, the characteristics of groundwater ages can be roughly estimated by summing values of travel distances and dividing by the velocity. Under this approach, the groundwater accommodated within the BVG at the Sellafield repository site was modelled to have a residence age between 60,000 and 250,000 years, and the trend is for the deeper waters to be older.

3.3.3 *Predicting the groundwater age through the particle tracking model*

To precisely date the groundwater age, the particle tracking model was used. Basically the migration of the particles would follow the streamlines according to the results of the particle tracking method. Two possible recharge sites were ascertained and both were investigated to predict likely groundwater ages. The travel time of the particles from one recharge site to the top of repository site is about 120,000 years following the upper and shorter stream line (Figure 6-9), the other is 140,000 years following the stream line through the repository site (Figure 6-10). The result of the modelling suggests that the residence age of groundwater at the repository site is at least 140,000 years. This is in extremely good coincidence with the stable isotope data ($\delta\,^{2}H$ and $\delta\,^{18}O$) for groundwater samples in the basement rocks of the repository site, which show that the recharge of basement rocks in the PRZ was derived from rainwater precipitation under colder climatic conditions before the last glacial period ended 10,000 years ago. The ^{4}He data give the maximum residence age of 1.6 million years (NIREX, 1995). Figure 6-9 shows that the particles arrive at the repository site after 140,000 years. Accordingly, the groundwater age at the repository site would be between 0.14 and 1.6 million years. The measured data of water residence age fit very well with simulation from a calibrated model of groundwater flow.

One of the most important reasons to date groundwater age is that we can validate the groundwater model through this process. Using the isotope data, or residence age, we can also retest the parameters used in the groundwater flow model, especially the very sensitive hydraulic conductivities of the BVG and the Granite. To approach this, we input several sets of permeabilities for the BVG and the

Granite, the results are given in Table 6.4. The effect of the permeability changes on predicting groundwater age is very significant, i.e., the groundwater residence age is very sensitive to the hydrogeological properties of the BVG and the Granite. Not only is the groundwater velocity altered by this, but also the flow path of the groundwater is altered as well (Figure 6-11, Figure 6-12). Thus using hydrogeochemical data is a very effective way to validate this regional groundwater model. It is also of interest to notice how the flow fields are influenced by the hydraulic conductivity of the BVG. The results from simulating the groundwater travel time indicate that the hydraulic conductivity of the BVG controls the residence age of the groundwater at the repository site. The modelling shows that the lower the permeability of the BVG is, the older the residence age of the groundwater will be. In addition to the velocity of the groundwater flow being influenced by the permeability of the BVG, its pathway is also changed dramatically as a result of this, and that causes the total traveling distance to vary from 4000 meters to 24,000 meters. If the hydraulic conductivity of the BVG is increased to 1.22 m/yr, the groundwater residence time would be only 3,000 years (Figure 6-11). That is too young and contradictory to the isotope data. This suggests that the average hydraulic conductivity of the BVG should be less than the 1.22 m/yr McKeown (1997) estimated. In the other extreme case, the hydraulic conductivity of the BVG was set one magnitude lower than the base value (Figure 6-12), and the flow field was altered greatly. As a result of this, the meteoric precipitation would not reach to the repository site which instead would draw water from Irish Sea Basin Regime. This conflict with the hydrochemical data measured in deep boreholes. These streamline contours also show that the basinal Brine Water regime would extend further east if the hydraulic conductivity of the BVG is set one magnitude lower than the base value (Figure 6-12). All these results imply that the hydraulic conductivity of the BVG should be constrained within the base value of 0.122 m/yr. What makes this striking is that the results of a geochemical calibration method are consistent with those of the sensitivity tests of hydraulic conductivity calibrated onto measured borehole pressures.

3.3.4 *Comparison of stream line method and dispersion method*

As was discussed before, the travel time of groundwater can be estimated simply by using a flow model and interpolating between computed isochron values. Travel distances are expressed as relative lengths along flow lines passing through the reference point (Toth, 1996). This method neglects the lateral dispersion of the element migration transported by groundwater flow and would inevitably cause an error in dating groundwater age. The errors resulting from neglecting dispersion are now analysed in this modelling and the comparison is made between the stream line isochron method and the particle tracking method. The prediction of groundwater travel time neglecting dispersion is illustrated in Figure 6-13. It is found that the groundwater travel time obtained by means of a stream line isochron is about 150,000 years at the repository site, 10,000 years older than the dispersion method, which means that the error is about 7% using the stream line isochron method.

4 RISK ASSESSMENT OF REPOSITORY SITE

4.1 Introduction

An important aspect for the safety assessment of a radioactive waste repository is the predictive modelling of the possible return time from radionuclide release in the future. The geosphere is one of the barriers in a multibarrier system for the isolation of nuclear waste in a geological repository. One reason behind the concept of disposing of nuclear waste in a geological repository is that the geosphere is relatively stable and time scales of geological processes are much longer than the characteristic time of human construction. Thus one would be taking advantage of the stability of the geosphere to provide the long term safety barrier for the nuclear waste. The geological barrier contributes to the final repository performance if, and only if, the likely transport of radionuclides through groundwater flow back to the biosphere is proved to involve a long time period, exceeding 10,000 to 100,000 years. The prediction of radionuclide migration aims to assess the safety of a natural barrier system which is one of the major components of a performance assessment for the long time periods required for disposal of radioactive nuclear waste. The effectiveness of this natural barrier is mainly controlled by the groundwater flow, through which the radionuclides are transported. Performance assessment for the disposal of nuclear waste is partly based on models which predict the evolution of the repository system and impacts that may occur thousands of years in the future. In this study, special large-scale hydraulic models have been developed to simulate the long-term evaluation of the groundwater flow field and distribution of fresh and saline waters. The model has been progressively validated (Chapter 4, Chapter 5 and Section 3 of Chapter 6) until there is confidence that the model is good enough to predict the long term safety of the repository site. Eventually the models should provide parameters for the consequent calculation of radionuclide transport in the geosphere.

4.2 Uncertainty analysis

Models are designed for use on systems that are more fully characterised than is achievable in practice at a real site. Satisfactory predictions from a model largely depend on the level of understanding, availability of information and data for a given site. Despite the wealth of appraisal data gathered in the Sellafield site characterization, the actual volume of rock that is represented by measurements is relatively small. The site characterizations are associated with several sources of potential errors and uncertainties regarding equipment, measurement technique, representivity, etc. Many of the parameters used in the site evaluation, e.g. hydraulic conductivity and dispersivity, cannot be directly measured but need to be estimated indirectly using interpretation models. Performance related models are frequently derived from the more complex models used to interpret real data measurements. Understanding of these performance models by means of models that aim at realism can assure that the simplifications do not give optimistic results and that field data are used appropriately. The ambition is to propagate all conceptual and other uncertainties that could not be resolved by the site characterization data and to evaluate their impacts on repository safety. However, there is no direct connection between site evaluation and the calculation of consequences. An important step is therefore to compile results of the site evaluation and model calculations in such a way that different sources of uncertainties can be evaluated. Another important aspect is to ensure consistency between parameters both within a discipline and between disciplines, e.g. between hydrogeology and geochemistry. The radionuclide transport calculations will in turn give feedback regarding the importance of different uncertainties in the models and required accuracy in the predictions made from the models. Herein after, these uncertainties are reviewed and analysed briefly.

4.2.1 *Hydraulic conductivity of rock*

Hydraulic conductivity is a vital parameter that controls the groundwater flow velocity and can be described by Darcy's Law (see chapter 3), the accuracy of hydraulic conductivity field measurement directly influences the accuracy of the prediction of the models. The determination of hydraulic conductivity has been fully investigated therein before, and the best fit suite of parameters were constrained to a unique set. In other words, the uncertainty of the hydraulic conductivity has been eliminated through the previous progressive tests.

4.2.2 *Flow velocity and path*

Transport calculations in performance assessments are based directly or indirectly on the flow characteristics. The groundwater flow velocity and the flow pathways during long time spans and large distances cannot be measured directly in the field, and therefore modelling provides a useful way to study these. The groundwater flow routes can be depicted by solving stream function equation and the features can be seen in the stream contour lines. Moreover, the origin of groundwaters can be indirectly evaluated from their chemical components which act as long lived natural tracers. This work has been tackled in Section 6.3 and the very important result is that the groundwater regime division based on its chemical components coincides with the flow divisions from modelling of groundwater flow, both flow rate and flux. Groundwater flow can also be calibrated via measured residence ages of groundwater, e.g. estimating groundwater age by means of a mass transport model and validating the model by hydrogeochemical data. As the groundwater at the repository site was found to be relatively old and recharged from the precipitation, so the flow path of the water should be modelled as long enough to take such long a time to travel. This event was reproduced via a particle tracking model and the result of the calculation agrees well with the isotope data.

The flow path was investigated independently from hydraulic conductivity sensitivity tests, instead of using the groundwater head data, however, it also uses chemical data to testify the origins of groundwater at Sellafield. Two sources of groundwater salinity were reproduced using the models and the two distinct flow regimes coincide with the two different hydrochemical components. The other important result from the flow path study is that the groundwater flow path at Sellafield is also very sensitive to changes in the hydraulic conductivity of the BVG. The basinal brine water system will intrude further into the repository site if the hydraulic conductivity of the BVG is decreased. Conversely, increasing the hydraulic conductivity of the BVG will cause a shorter flow path of groundwater at the PRZ and consequently a much younger residence age of the water. The striking point after this test is that a reasonable parameter for the actual flow regime is obtained and it coincides with the value obtained by calibration to measured head data in Chapter 4.

4.2.3 *Dispersivity*

The other important parameter upon which the mass transport relies is the dispersivity, and that has been addressed by introducing the equations of advection and dispersion. See equation (6-1) and equation (6-3). For porous media, the typical rationale is the need to know the flow and transport porosity, together with the quantification of dispersion. The true dispersion of flow in these rocks is not known, there has not been a field tracer experiment undertaken at this stage of the site characterization. Consequently the only way to investigate dispersivity in the risk assessment of the radioactive nuclear waste repository site at this moment is via modelling. It has been suggested that the identification of such slow processes of natural dispersivity is better accomplished in the domain of natural analogue studies, rather than of field tracer tests (OECD, Field Tracer Tests, 1996).

A typical range of values in longitudinal dispersivity from experimental column experience is from 10^{-2} to 1 cm (Domenico *et al,* 1990). In field experiments, values range from 0.1 to 2m over relatively short distances (Domenico *et al*, 1990). In media with pronounced horizontal stratification, values of vertical dispersivity may be similar to the bulk diffusion coefficient (about 10^{-6} - 10^{-4} cm^2/s). Table 6.4 gives some dispersivity values based on tracer tests. In NIREX modelling work, a steady-state model using the NAMMU finite-element code was developed to investigate the dispersion required to match the inferred saline transition zone. The hydrodynamic dispersion was incorporated directly. Using a constant salinity at the western boundary of the model, corresponding to six times sea-water concentration, the main features of the saline transition zone were reproduced with the dispersion length of 30m and a transverse dispersion length of 1 m. (NIREX, 1993)

To estimate the dispersivity of the rocks at Sellafield, sensitivity tests of dispersivity were carried out and the effects of these on the predictions are analysed. The results of some of those tests are illustrated in Figure 6-14, and they are summarised below.

1) Dispersivity of the rocks at Sellafield has a significant effect on the migration of radionuclides from the repository site. Longer travel distances are more affected.

2) Figure 6-14 shows that dispersion of transport makes the distribution of radionuclides widespread during their migration. If higher dispersivity is assigned for these rocks, a broader transition zone of the radionuclides will form.

3) Although predictions of radionuclide migration are influenced by the dispersivity of rocks, final travel times from the underground disposal site back to the surface under various dispersivities are very little changed, they are in the same order of magnitude, around 50,000 years.

4) Varying dispersivity of rocks at Sellafield has very little impact on radionuclide migration, based on the sensitivity tests. This is not a critical feature, and so the safety of the repository site can be assessed using the transport model inputting the average parameters of dispersion.

4.3 Predictions

With uncertainties of appropriate rock properties being reduced by calibration, it is now possible to make predictions using the model, utilizing those appropriate rock properties. These parameters are set out in Table 6.4. The sorption coefficient is taken as 1 for conservative prediction.

The prediction of the radionuclides are made presuming that these radioactive wastes somehow escape from the capsule of the drum and steel barrels, and participate in the migration of groundwater. The migration of radionuclides is illustrated in Figure 6-15. Most of the radionuclides released from the disposal site will be transported further west towards the offshore. The travelling time of the radionuclides in the subsurface mainly depends on their travel distance, groundwater flow velocity and dispersivity. Table 6.6 contains the summarised predictions from the model. The migration route and the distance of their travelling are seen in Figure 6-15, which can be identified as these stages:

—Firstly, all the escaped radionuclides would migrate in the BVG close to the PRZ.

—Secondly, these radionuclides pass into Sherwood Sandstone Group after 3,000 years.

—Thirdly, after about 25,000 years, they arrive at the Calder Sandstone aquifer.

—At last, some of them will reach the sea water of East Irish Sea in about 50,000 years.

The most important stages of the migration are described as follows:

4.3.1 *Migration in the BVG*

Based on the stream lines calculated from the models, the travel path of radioactive waste in the BVG is about 800 meters. To travel through this distance will take 2,000–3,000 years for the radionuclides.

4.3.2 *Migration through Permian into St. Bees Sandstone*

Since the Permian at the Sellafield is only about 50 meters thick, the radionuclides will go through it within 500 years and the radionuclides will soon reach the St. Bees Sandstone after their voyage in the BVG, roughly 3,000 years since release.

4.3.3 *Migration into the Calder Sandstone (aquifer formation)*

The distance of migration for the nuclide transport provided in the St. Bees Sandstone is between 1,500 m and 2,000 m, so the time to be taken for the migration is between 20,000 years and 25,000 years. The depth of these particles will be 400 m bOD when they enter into the Calder Sandstone.

4.3.4 *Migration to the surface*

Once the radionuclides reach the Calder Sandstone, they will pervade through the more than 700 m thick Sandstone aquifer and the travel distance varies from 1,500 m to a few kilometers. A minority of these traveling radionuclides might take the short distance and return to the biosphere within around 50,000 years, at a location about 1 km west of the coast. However most of them will travel a much longer distance towards the west beneath the East Irish Sea.

4.3.5 *Migration under different dispersivities*

As no field tracer test has been undertaken at Sellafield, these predictions might be impacted by variations in dispersivities of the rocks. It is necessary to assess the effects of variance of dispersivity on the prediction. To fully understand the influence of this, prediction through the model was carried out using three sets of dispersion parameters, one set is the average value, based on other workers (Table 6.3), the others are one order of magnitude higher or lower than the average respectively. The results of these predictions are shown in Table 6.6. From the derivation of dispersion and diffusion equations in Section 2, we know that the dispersion is the additional flux resulting from the fluctuating velocity and causing the spreading. Since groundwater flow at Sellafield is towards the west at a very gentle angle, the dispersion will cause significant spreading of its distribution horizontally rather than vertically. It can be seen that both the travel distance and travel time are reduced when the dispersivity is increased. In this modelling, the vertical dispersivity was assigned as one tenth of the longitudinal dispersivity. The values of vertical dispersivity may well be less than that and may be similar to the bulk diffusion coefficient (Domenico, 1990). Consequently, the final return time for the radionuclides from the disposal site back to the surface would be between 50,000 years and 80,000 years.

5 CONCLUSION

From the analysis and investigation of hydrogeochemical data in deep boreholes at Sellafield, the predicted flow field is coincident both with measured data and the conceptual model. The characteristics of groundwater flow have been linked with the successful reproduction of a groundwater flow field. Therefore the predictions of radionuclide migration using this calibrated mass transport model should be reasonable. Accordingly, these conclusions can be drawn:

1. The flow path of groundwater was reproduced using the models. The modelling produced two distinct flow regimes, and these coincide with the two different measured hydrochemical components. The groundwater flow path through the repository site originates from precipitation in mountain areas 16 km to the east. The flow path from the repository extends to reach the surface in the Sherwood Sandstone Group 4 km to the west.

2. Based on groundwater flux and its route, the groundwater flow system can be divided into: 1) A Shallow Flow Region that has a short travel distance and a large flux, 2) an Inland Flow Region with a long travel distance but small flux, and 3) an Irish Sea Basin Region which has little flux.

3. From this modelling, there are two sources of salinity in groundwater at Sellafield, one is the Inland Flow Region resulting from water and rock interaction in the east; and the other is the Irish Sea Basin Region from the dissolution of halite in the west. This is coincident with measured geochemical data.

4. The groundwater residence time modelled at the proposed repository site is at least 0.14 million years. The deeper groundwaters have older ages. These are coincident with geochemical data.

5. Isotopic measurements of groundwater residence age show that groundwater in the PRZ is older than 30,000 thousand years, and younger than 1,500, 000 years. Results of modelling suggest that the residence age of groundwater at the repository site is at least 140,000 years. This is quite well in agreement with the stable isotope data ($\delta\, ^2H$ and $\delta\, ^{18}O$) for groundwater samples in basement rocks of the repository site, which shows that the groundwater of the basement rocks of the

PRZ was recharged into the flow system under colder climatic conditions before the last glacial period that ended 10,000 years ago.

6. Both the hydraulic parameters of the rocks and flow lines of groundwaters can be calibrated using chemical and isotopic data measured from deep borehole samples, which agree with the results of sensitivity tests via the groundwater head data discussed in Chapter 4. Validation of mass transport models via dating the groundwater indicates that the hydraulic conductivity of the BVG also controls the residence time of groundwater at the repository site. It is suggested that the hydraulic conductivity of the BVG is 0.12m/yr. This is less than the 1.22 m/yr proposed by McKeown (1997).

8. It is found that the groundwater travel time obtained by means of stream line isochrons is about 150,000 years at the repository site, 10,000 years older than suggested by the dispersion method, which means that the error is about 7% using the stream line isochron method.

9. Predictions from this modelling suggest that the radionuclides that may be released from the repository site will migrate underneath the East Irish Sea. Only a minority of them will reach to the seabed. The return time for radionuclides released from the PRZ site to the surface of the sea bed of the East Irish Sea, is between 50,000 years and 80,000 years, 3 km west away from the PRZ. But these radionuclides will arrive at the Calder Sandstone aquifer at a depth of 400 m in about 25,000 years, 2 km west from the PRZ.

6 SUMMARY

Numerical modelling of radionuclide transport provides an insight into groundwater movement. Transport calculations in repository performance assessments are based directly or indirectly on the groundwater flow characteristics. Still there are uncertainties in the basis of transport modelling. It is critical to choose suitable parameters to feed into the model of mass transport in groundwater. The previous numerical modelling of Sellafield was performed by a number of organizations working together (Heathcote et al. 1996), with emphasis on reproducing the groundwater head at the repository site. None of their work was involved in simulating radionuclide transportation. In this present study, the migration of groundwater from recharge areas to the repository site was simulated using OILGEN's mass transport computer program, and both dynamic dispersion and molecular diffusion are involved in the study. In general, all the transport models are based on the principle of conservation of mass. Advection and dispersion are regarded as being the major phenomena transporting any radionuclides leaching from the nuclear waste repository. The flow-rate of water in the ground is calculated by Darcy's law and the transport of solute is denoted by the so-called advection-dispersion equation.

The advection-dispersion transport equation is more difficult to solve numerically than the flow equation. The advantage of the random walk method particularly is that it performs well for large Peclet numbers. The other advantage of the random walk method is that it conserves mass, even if the flow field is not computed with high precision, and it may not require the solution of large systems of equations. This method is well suited for this study because even small quantities of radioactive waste leakage are vital in the assessment of potential migration away from the storage site. In predicting radioactive waste migration, what we want to understand is the first arrival of the nuclides. To this end, the particle tracking method is the most effective means to implement in helping us to investigate it.

The variation of salinity was observed and calculated from the field measurements, either from total dissolved solid values for the groundwater samples, or from the basis of electrical conductivity data. There might be two sources of salinity. All the differences between groundwater chemical components acting as natural tracers reveal that the origins of them are different. The major basinal component is in Borhole 3 at the coastline; the inland component is dominant in Borehole 2 at the PRZ; a mixture of the components is in Borehole 10A in the middle. This two component mixing phenomenon is well reproduced in this modelling. The most striking point is that the flow regime derived from groundwater flow modelling agrees well with the separated, independent, data from distribution of measured chemical data.

The stable isotopes ($\delta\,^{2}$H and $\delta\,^{18}$O) for groundwater samples in the basement rocks of the repository site have meteoric signatures. The stable isotopic signatures and recharge temperatures derived from noble gas abundances in the groundwater samples indicate that recharge conditions for groundwaters in the BVG of the PRZ were colder than those in the sandstones. Both stable isotope compositions and inert gas contents depend on climatic conditions at the time of recharge, and all these indicate that the recharge of basement rocks in the PRZ was under colder climatic conditions before the last glacial period ended 10,000 years ago.

The groundwater age can also be estimated by investigating groundwater travel times using groundwater flow model (Toth and Sheng, 1996). This modelling of groundwater reveals that the groundwater in the repository site is recharged from the precipitation in the mountain area, and the groundwater residence time at the proposed repository site is at least 0.14 million years. That is coincident with the measured geochemical data from ^{14}C, He, $^{36}Cl/Cl$ which indicate that groundwater at PRZ is older than 30,000 years and younger than 1.5 million years.

Site characterization is associated with several sources of potential errors and uncertainties. Many of the parameters used in the site evaluation, e.g. hydraulic conductivity and dispersivity, cannot be directly measured but need to be estimated indirectly using interpretation models. One approach to the problem is to use hydrogeochemical data as long lived natural tracers to determine effective transport parameters directly. Since the location of recharge of the groundwater at the repository site has been determined, a more effective method of determining transport parameters directly is by fitting models to data of groundwater age. Both the hydraulic parameters of the rocks and the flow lines of groundwaters can be evaluated using chemical data, and the results agree with the independent results of sensitivity testing via the data of groundwater head discussed in Chapter 4.

It is found that the groundwater travel time obtained by means of stream line isochrons is about 150,000 years at the repository site, 10,000 years older than the dispersion method implies, which means that the error is about 7% using stream line isochron method.

With these uncertainties fixed, it is possible to make predictions under defined circumstances. Firstly, nuclides would migrate into the BVG, then pass into the Sherwood Sandstone Group after 3,000 years; secondly, after about 25,000 years, they can arrive at the aquifer of the Calder Sandstone. At last, some of them will reach the sea water of the East Irish Sea in about 50,000 years. Most of the radionuclides released from the disposal site will be transported west towards the offshore under the sea bed of the East Irish Sea.

The success of a model in reproducing the measurements of field exploration, groundwater head and chemical data, builds confidence that relevant features and processes have been identified. Characterization of hydrogeology is the main task at a potential disposal site and performance assessment has to rely on the relations between the hydraulic and transport properties, and identification of uncertainties.

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EXPERIMENTS	MIGRATION DISTANCE (m)	DISPERSIVITY (m)	FISSURE WIDTH (m)
Laboratory with natural fissure (Neretnieks etc. 1982)	0.3	0.025	0.18
Laboratory with natural fissure (Moreno, etc. 1984)	0.27 0.19	0.011 0.005	0.14 0.15
Stripa natural fissure, two different channels (Abelin, etc. 1982)	4.5 4.5	2.0 0.62	0.11 0.14
Finnsjon site (Moreno, etc. 1984)	30	0.35/5	0.47-0.98
Studsvik site (Landstrom, etc. 1978)	22 51	0.1 7.7	
French site (Lallemand-Barres, 1978)	11.8	0.8	
Spain El Berrocal site, granite (J. Guimera etc. 1996)	22	1.6 2.7	$0.2X10^{-3}$
Laboratory single rock fracture, slate. (K.A.Cliffe, etc. 1993)	1.05	0.05	$0.65X10^{-4}$

Table 6-3 Dispersivities from tracer tests in fractured rocks

Depth	***m bOD***	***200-223***	***317-323***	***360-364***	***543-555***	***711-721***	***1011-1026***	***1587-1602***
Formation		St. Bees	St. Bees	St. Bees	BVG	BVG	BVG	BVG
Lithology		Sandstone	Sandstone	Sandstone	Tuff	Tuff	Tuff	Breccia
Temperature	°C	13.1	15.1	15.5	20.5	22.9	31.5	45.4
pH	$\log\{H^+\}^*$-1	<7.25	<7.35	<8.26	<6.25	<6.52	<7.85	<7.14
Eh	mV	<355	360	<11	46	<66	90	92
Conductivity	mS/cm@20°C	0.296	0.295	0.382	38	36.6	44.7	47.1
Sodium	mg/l	12.8	29.1	8616	8000	7500	8530	9120
Patassium	mg/l	1.91	2.81	5.49	102	95.8	151	187
Calcium	mg/l	32.6	24.4	11.7	685	484	1080	1490
Magnesium	mg/l	11.4	15.3	4.3	82.3	62	150	136
Chloride	mg/l	12	25.2	10	13000	12600	15700	17400
Sulphate	mg/l	9.15	6.8	16.7	1060	962	1210	1130
Bromide	mg/l	0.101	0.059	0.103	23.6	22.1	25.9	30.3
TDS	mg/l	191	179	251	24300	23100	28400	30000
$\delta^{18}O$	per mil (SMOW)	-6.1	-6	-6.1	-7.6	-7.5	-7.5	-7.7
$\delta^{2}H$	per mil (SMOW)	-36.4	-34.4	-36.2	-41.7	-41.2	-43.6	-45.9
Tritium	TU	3.5	2.9	4.2	2.4	1.9	1.5	0.8
Recharge Temperature	°C	10.9	18.6	9.9	6.7	7.1	6.8	5.2

Table 6.1 Geochemical Data In Borehole 2: (Selected from Nirex Report No 524)

Depth m bOD **Formation** **Lithology**	*573-640* **St. Bees** **Sandstone**	*692-700* **St. Bees** **Sandstone**	*776-782* **St. Bees** **Sandstone**	*931-941* **St. Bees** **Sandstone**	*1108-1118* **St. Bees** **Sst with muds**	*1538-1555* **Carboniferous** **Limestone**	*1671-1682* **BVG** **Tuff**
Temperature °C							
pH log{H$^+$}	-	7.79	7.53	6.69	7.22	6.47	7.31
Eh mV	-	158	222	112	-12	72	40
Conductivity mS/cm@25°C	52.7	122	136	163	193	157	203
Sodium mg/l	10700	41900	44500	57300	71600	49300	65100
Potassium mg/l	62.8	241	302	329	327	292	539
Calcium mg/l	598	2320	2270	2650	2520	2610	2910
Magnesium mg/l	413	494	465	585	686	537	489
Chloride mg/l	16400	64200	65800	85800	108000	77700	104000
Sulphate mg/l	990	3580	3640	4430	4910	4740	3340
Bromide mg/l	19.1	65.4	69.1	82.4	96.6	78	108
TDS mg/l							
$\delta^{18}O$ per mil (SMOW)	-7	-6.3	-6.3	-5.5	-5.1	-5.8	-5.9
$\delta^{2}H$ per mil (SMOW)	-46.9	-44.2	-43.4	-37.7	-32	-41.7	-32.1
Tritium TU							
Recharge Temperature °C	8.1	10.8	13.5	-	20.8	16.3	-

Table 6.2 Geochemical Data In Borehole 3: (Selected from Nirex Report No 524)

Lithology	Hydraulic properties				Thermal Properties	Dispersion properties		
	Permeability (millidarcy)	Hydraulic conductivity (m/yr)	Anisotropy Kh/Kv	Porosity %	Thermal Conductivity (cal/m sec °C)	Longitudinal Dispersivity (m)	Vertical Dispersivity (m)	Diffusion Coefficient ($10^{-8}m^2/yr$)
Glacial Drift	10	2.99	10	1.5	1	20	2	1
Calder Sandstone	10	2.99	10	1.5	1	20	2	1
St Bees Sandstone	3	0.93	10	1.2	1	5	0.5	1
Permian	0.004	0.0012	20	0.01	0.7	0.1	0.01	1
Carboniferous Limestone	4	1.24	1	0.1	0.8	5	0.5	1
BVG	0.4	0.12	5	0.1	0.7	2	0.2	1
Skidaw Group	0.04	0.012	15	0.08	0.6	0.1	0.01	1
Granite	0.03	0.009	0.5	0.02	1.5	1	0.1	1
Fault in BVG	0.5	0.155	0.2	1	0.5	10	1	1
Fault in Sandstone	5	1.55	0.5	1.6	0.8	30	3	1

Table 6-4 Final validated parameters used in the models

Lithologies met by the radionuclides	**Travel distance from the PRZ** (km)	**Travel time** (yr)
Permian	0.5-0.9	2,500
St. Bees Sandstone	1-1.5	3,000
Calder Sandstone	2-2.5	25,000
Biosphere	>3	50,000

Table 6.5 Prediction of radionuclides transportation into different lithologies (yr.):

Lithologies reached by radionuclides)	**Travel time under lower dispersivity** ($a_L = 0.1$ m)	**Travel time under average dispersivity** ($a_L = 2$ m)	**Travel time under higher dispersivity** ($a_L = 50$ m)
Permian	2,500	2,500	2,,000
St. Bees Sandstone	3,000	3,000	2,500
Calder Sandstone	30,000	25,000	20,000
Biosphere	80,000	50,000	30,000

Table 6.6 Prediction of radionuclides transportation from different dispersivity (yr.):

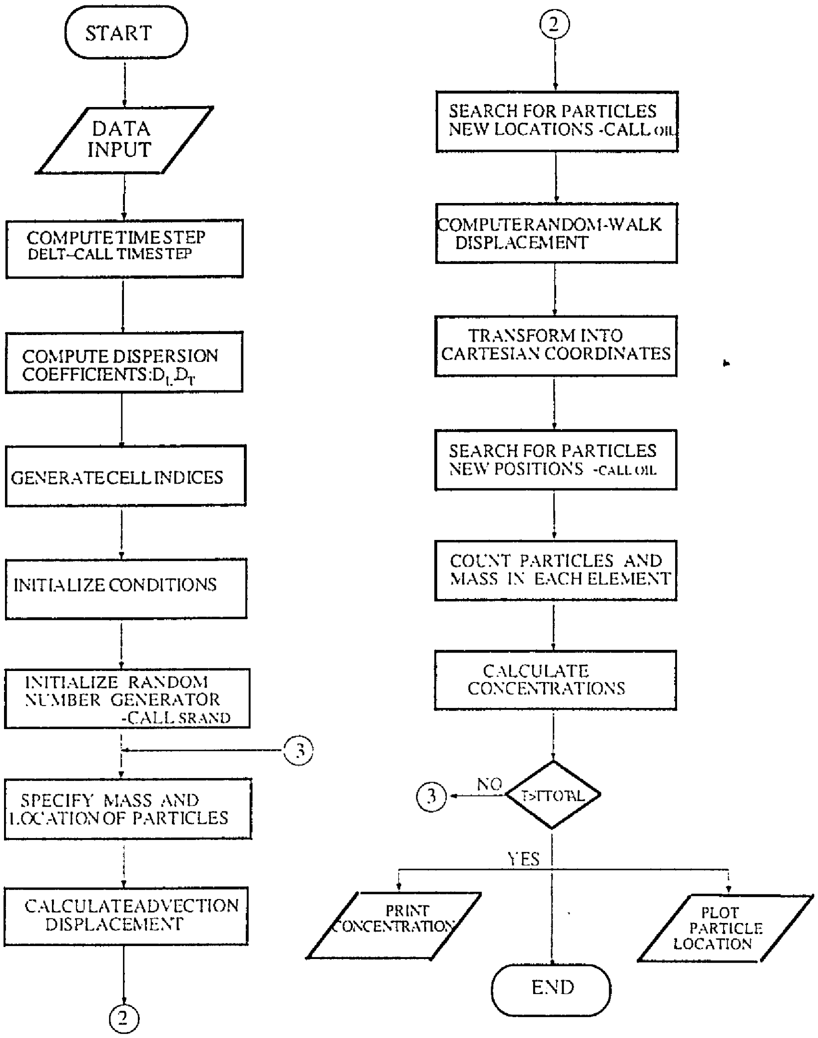


Figure 6-1 The flow chart of the mass transport model

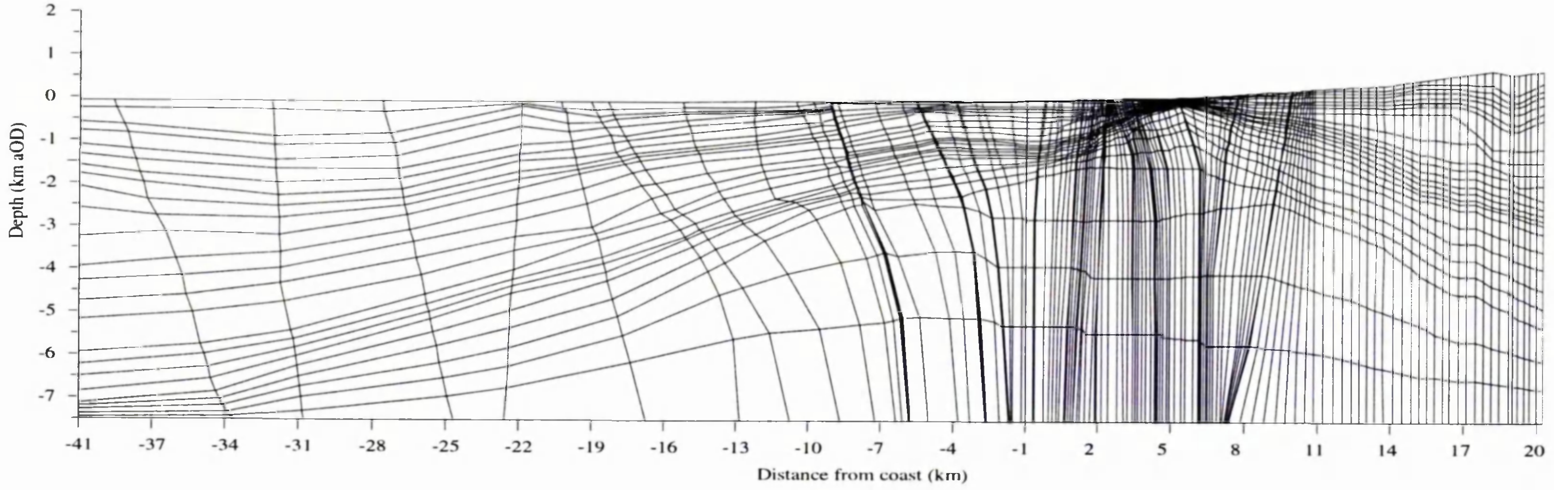


Figure 6-2 Quadrilaterals used in mass transport model

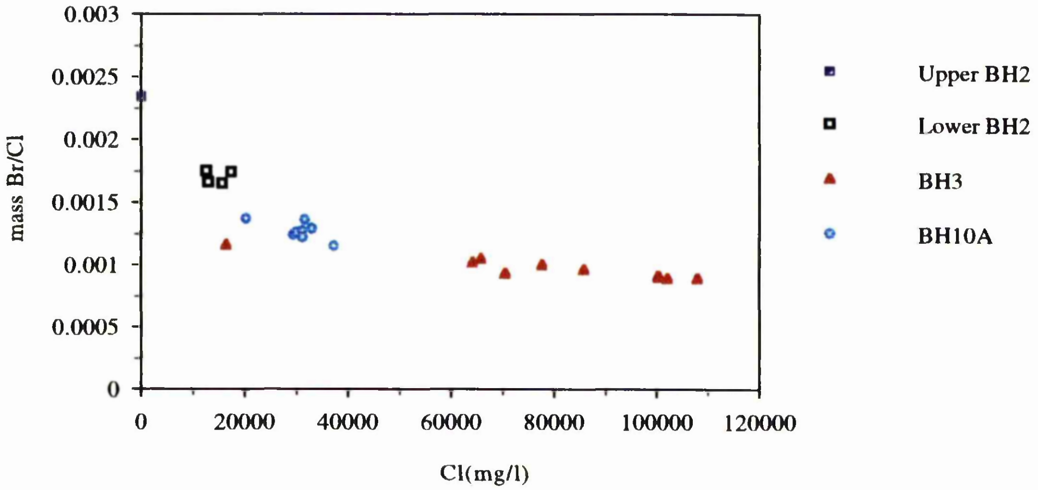


Figure 6-3 Br/Cl versus Cl for the deep borehole groundwaters (replot from Nirex data)

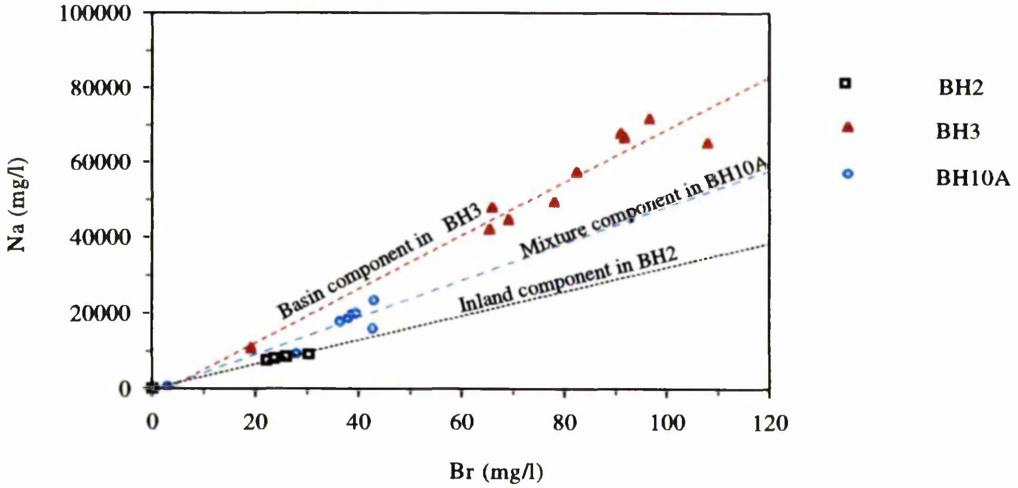


Figure 6-4 Na versus Br plot for the deep borehole groundwaters (replot from Nirex data)

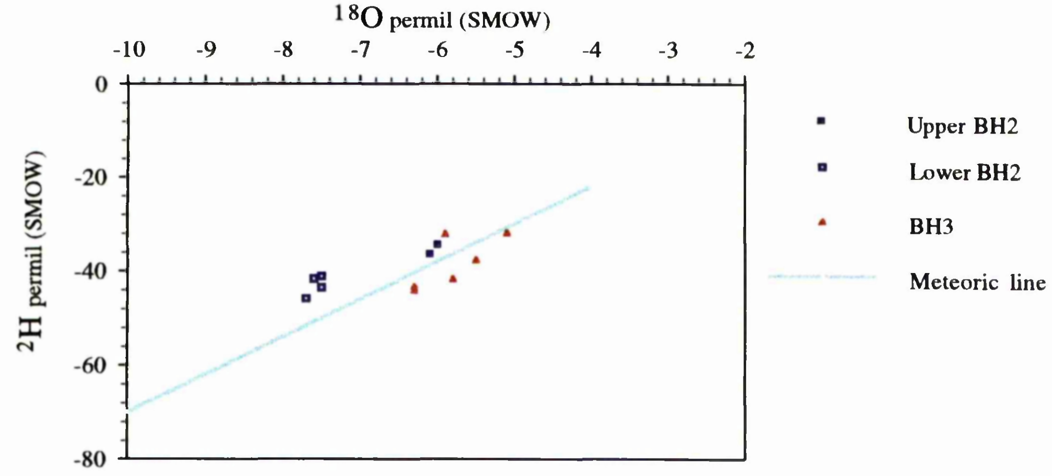


Figure 6-6 Stable isotope plot for the deep borehole groundwaters (replot from Nirex data)

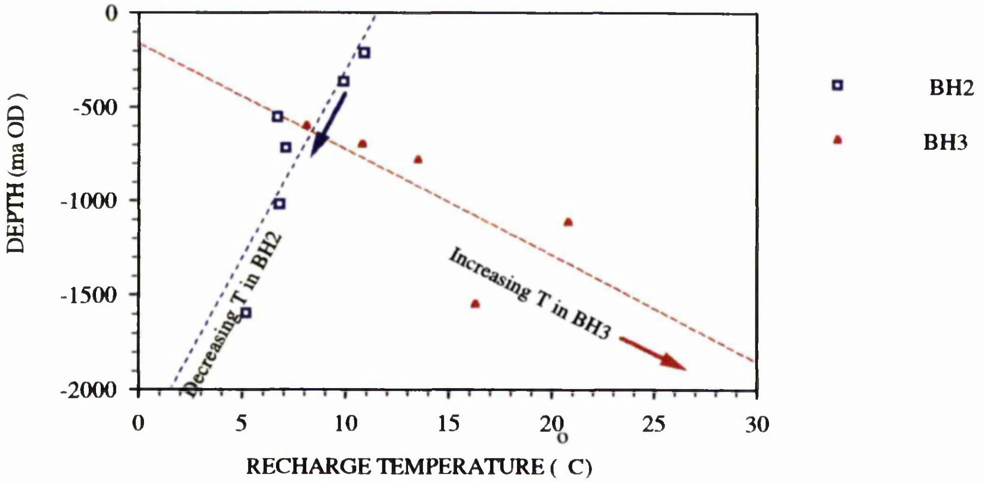


Figure 6-7 Recharge temperature versus depth plot for the deep borehole groundwaters (replot from Nirex data)

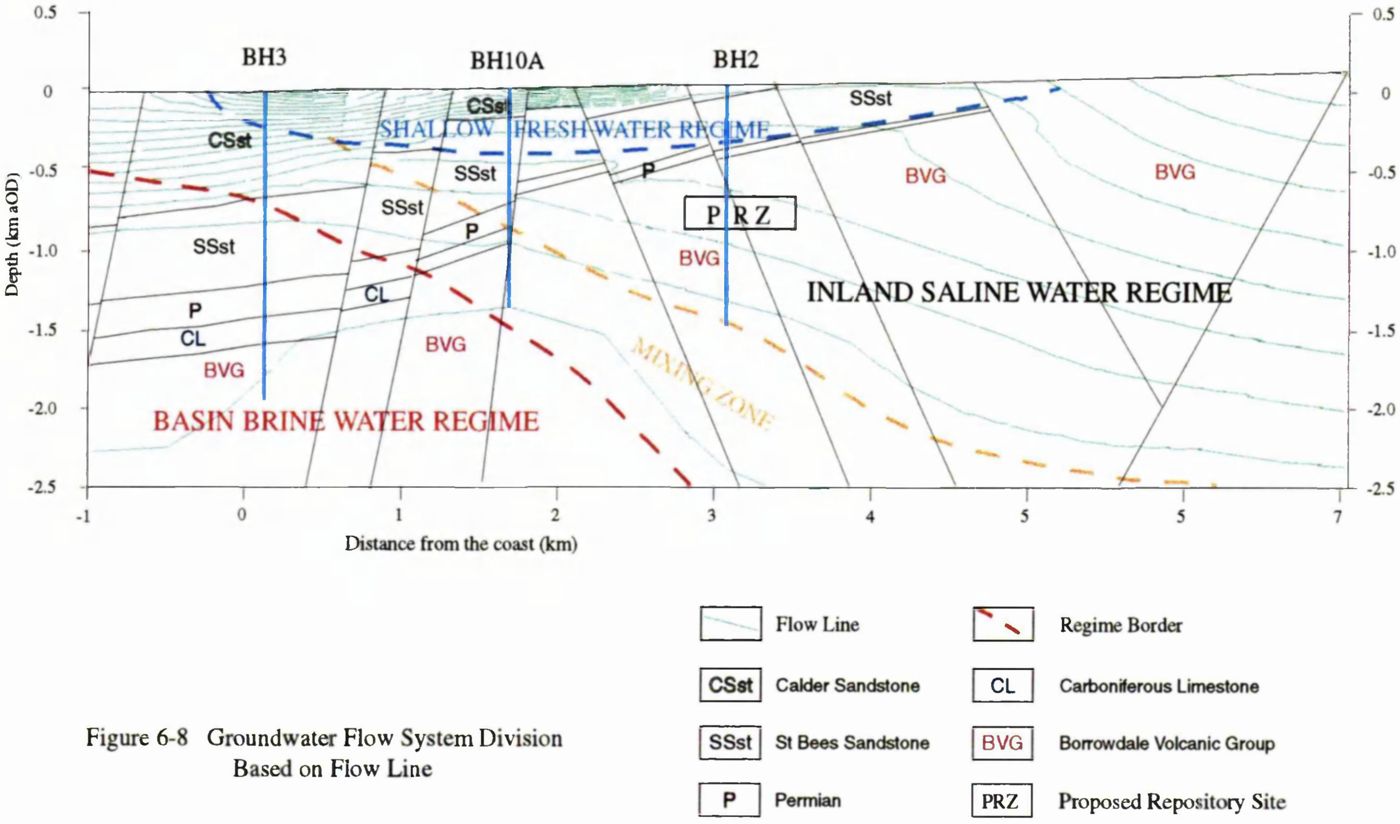
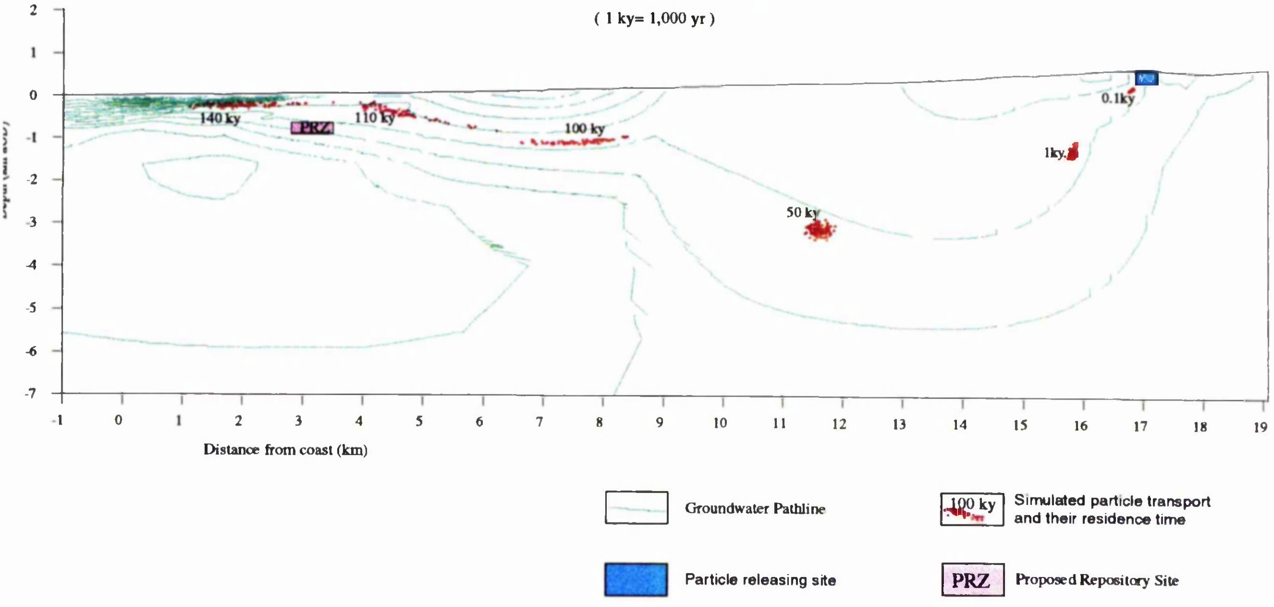


Figure 6-8 Groundwater Flow System Division Based on Flow Line

(A) Groundwater travel time /short path



(B) Groundwater travel time /long path

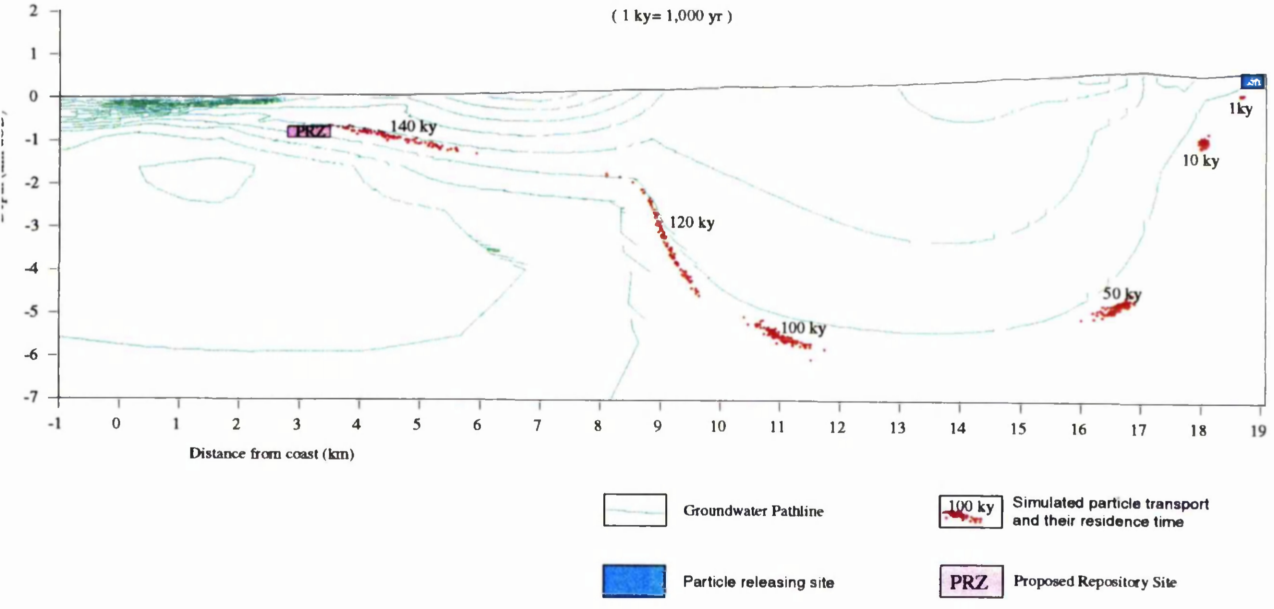
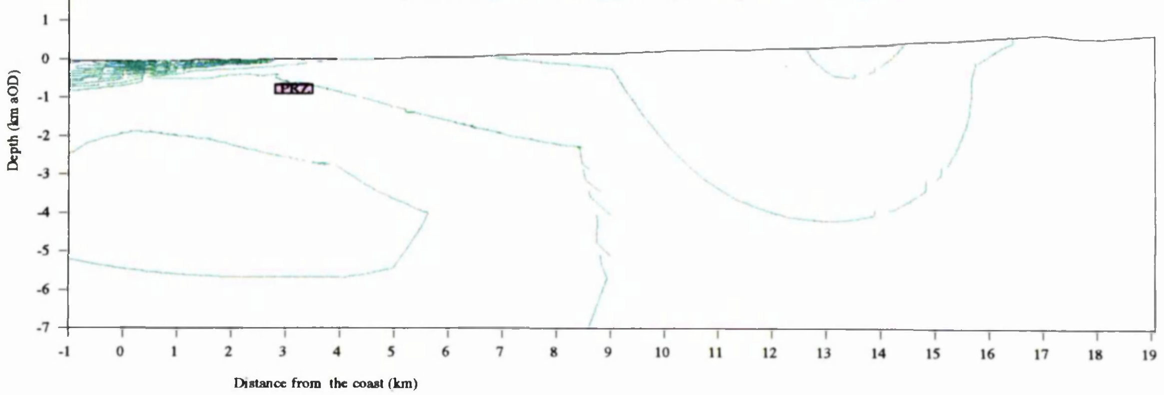
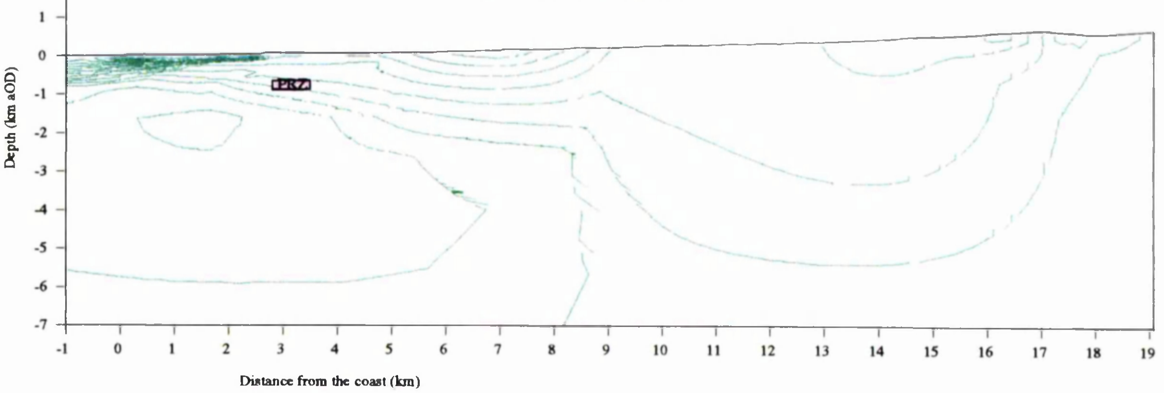


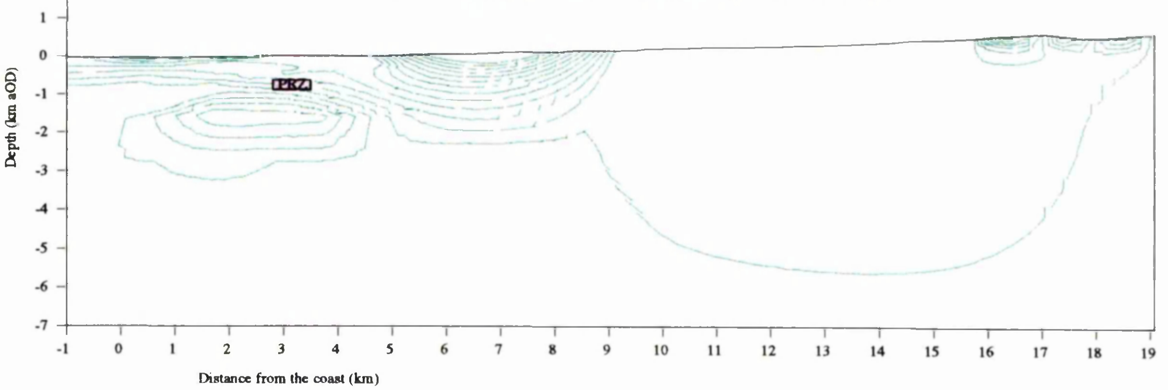
Figure 6-9 Groundwater travel time predicted from the model: (A) shows particles released from near site and travels along a short distance. By contrast, (B) shows a long distance of travelling


(A) Stream line from the lower hydraulic conductivity of BVG

The hydraulic conductivity of the BVG=0.012 m/yr, one magnitude lower than base value


(B) Stream line from the base value

The hydraulic conductivity of the BVG = 0.12 m/yr


(C) Stream line from the higher hydraulic conductivity of BVG

The hydraulic conductivity of the BVG = 1.2 m/yr, one magnitude higher than base value

Figure 6-10 The groundwater flow lines vary with different hydraulic conductivities of the BVG

(A) and (C) shows the flow pathline will not reach the PRZ if the hydraulic conductivity of the BVG is either 0.012 m/yr (lower than the base value), or 1.2 m/yr (higher than the base value).

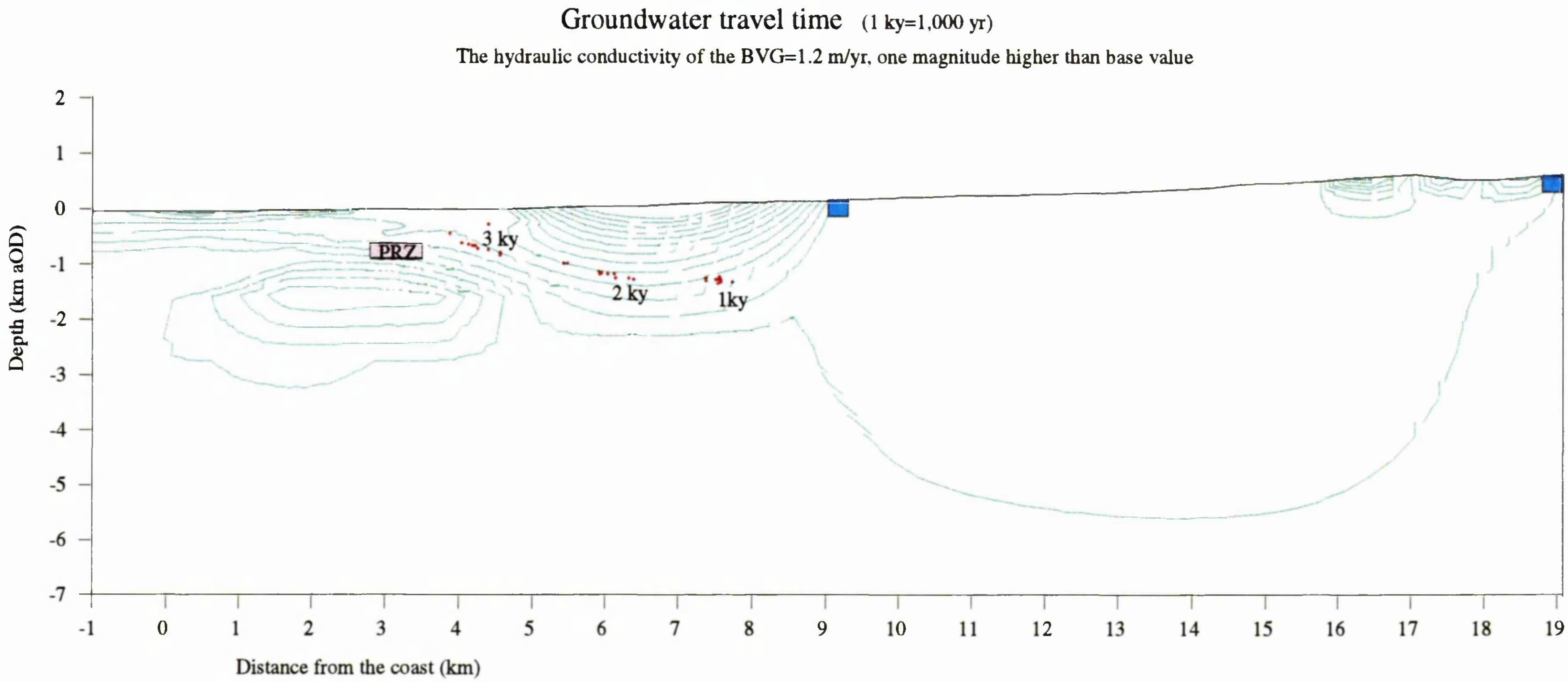


Figure 6-11 Groundwater travel time predicted from the model

The time of groundwater travel will be very short, only a few thousand years,
as a result of higher hydraulic conductivity of the BVG,
if the hydraulic conductivity of the BVG=1.2 m/yr, one magnitude higher than base value

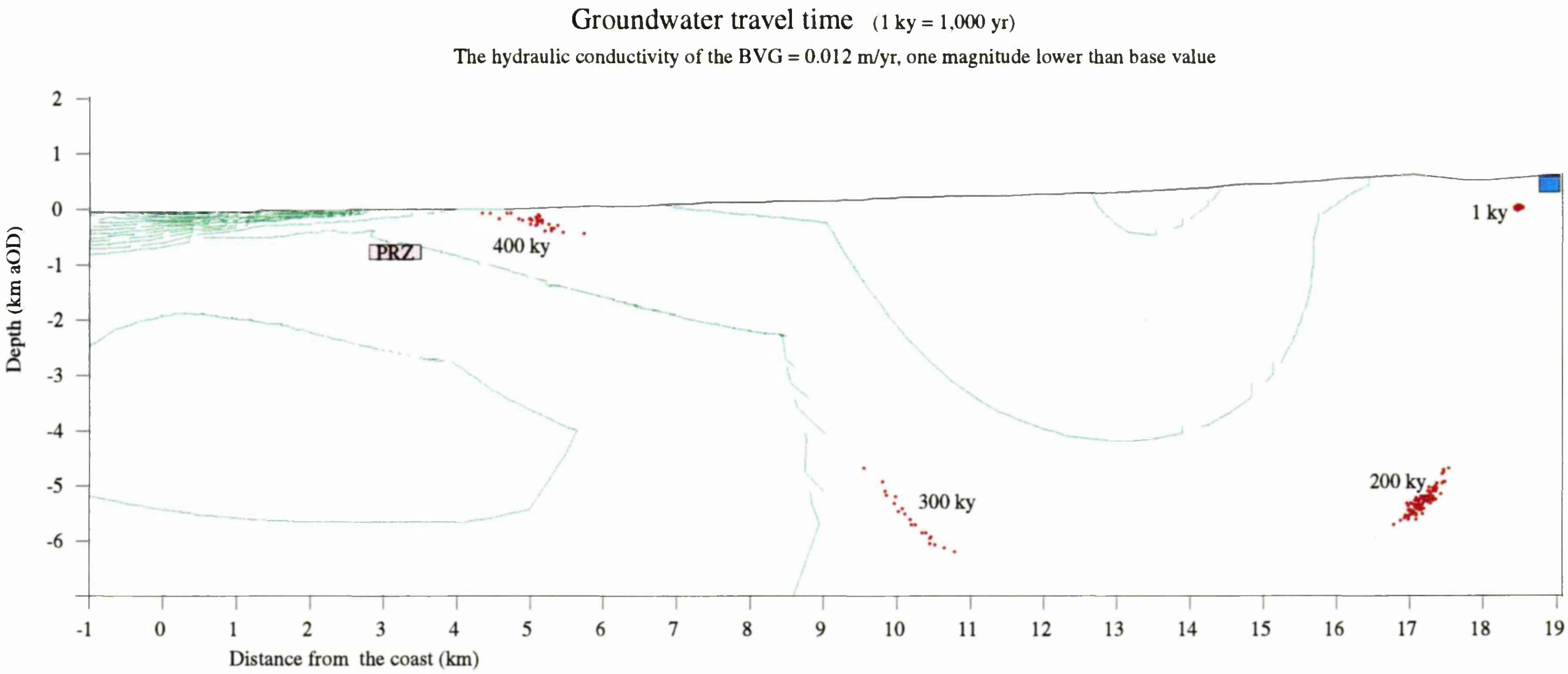


Figure 6-12 Groundwater travel time predicted from the model

The groundwater from the precipitation will never reach the PRZ,
as a result of lower hydraulic conductivity of the BVG,
if the hydraulic conductivity of the BVG = 0.012 m/yr, one magnitude lower than base value

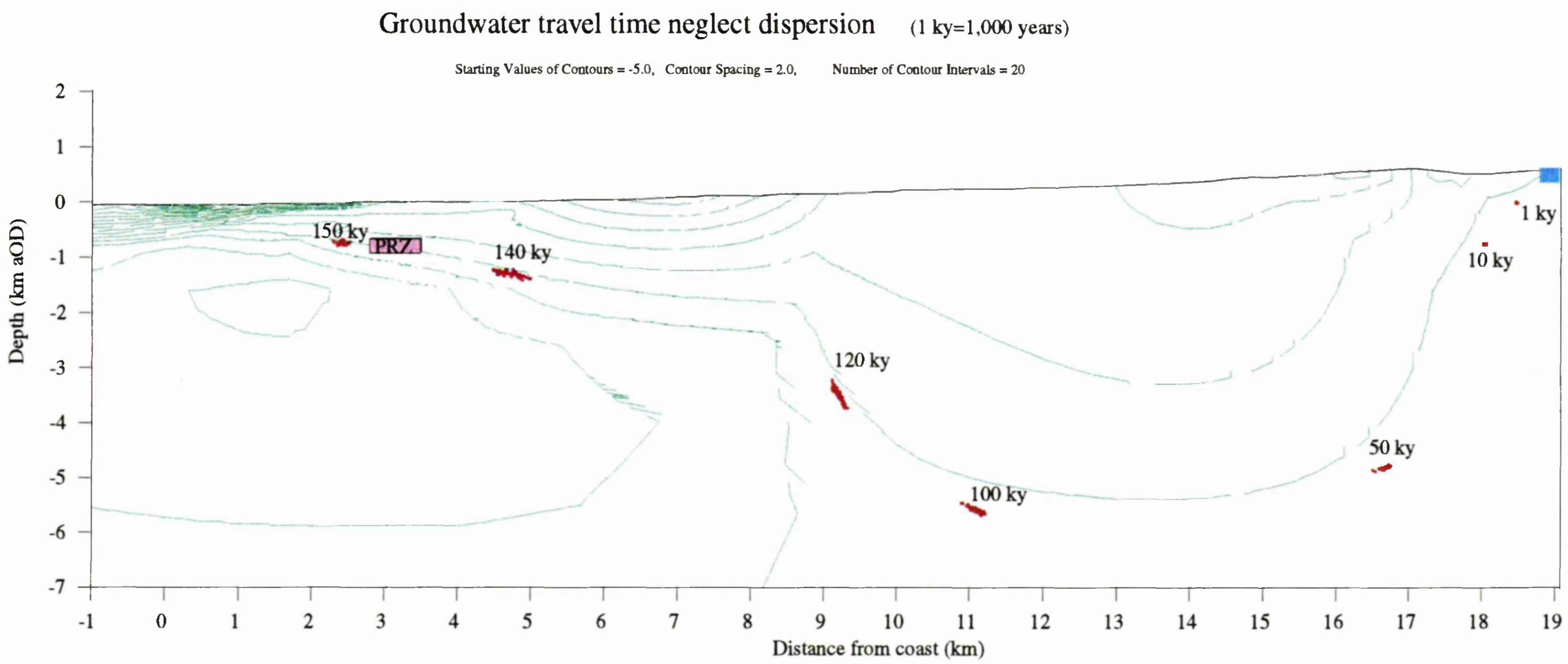


Figure 6-13 Groundwater travel time neglect dispersion

As a result of neglection of dispersion, the time of groundwater travel will be 10,000 years (about 7%) sooner.

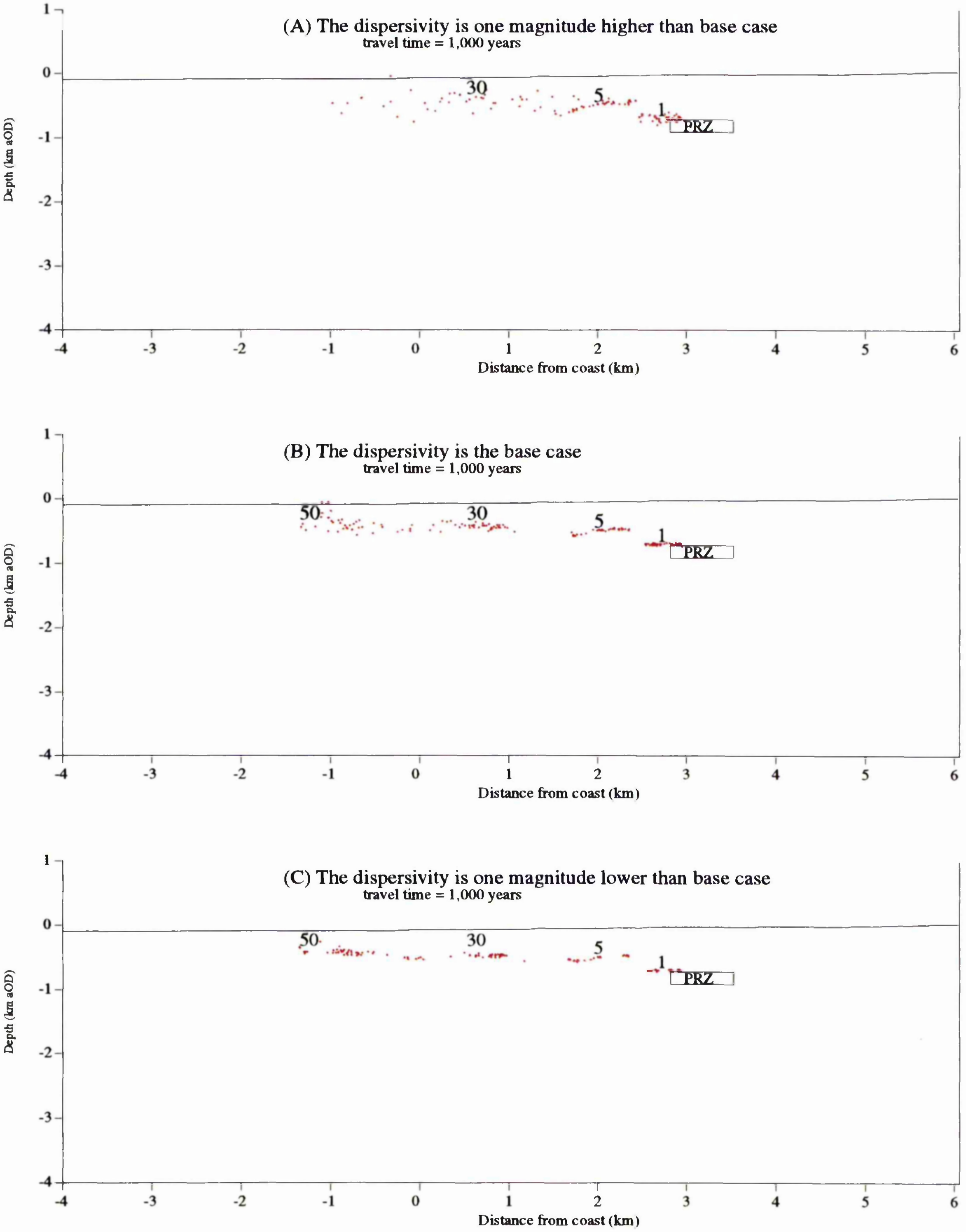


Figure 6-14 The predictions of radionuclides migration under various dispersivities

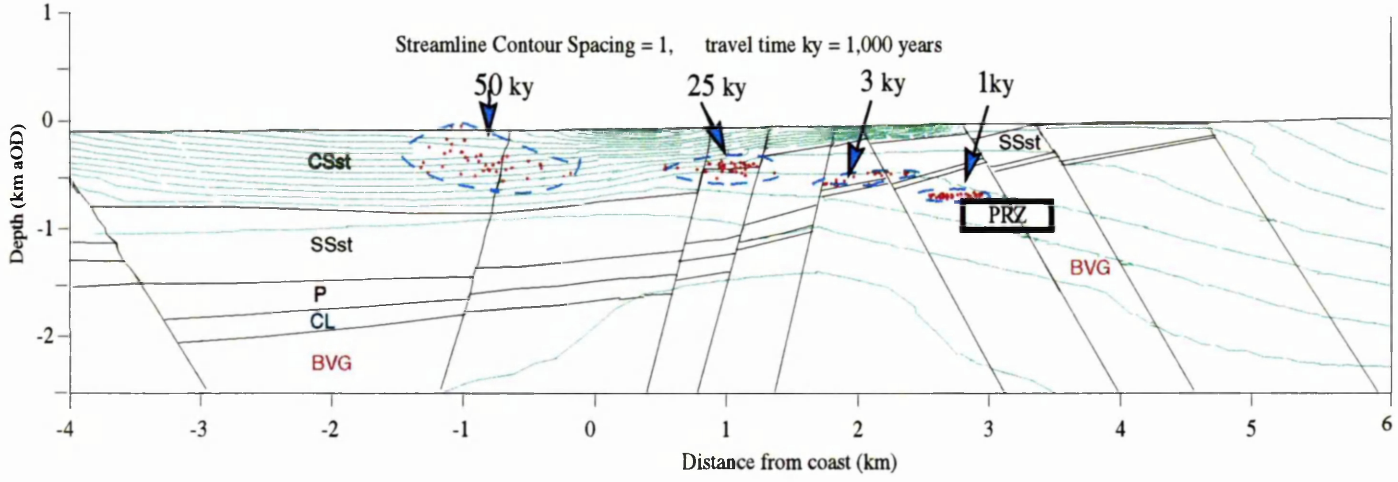


Figure 6-15 Prediction of Radionuclides Migration Time

It shows that the radionuclides will go into the Calder Sandstone by 3 thousand years, reach to the sea bed about 50,000 years

Chapter 7

DISCUSSION AND CONCLUSION

When this Ph.D. research commenced, modelling groundwater flow at Sellafield was still at an early stage. There were gaps to be filled in explaining the specific characteristics of the groundwater system at Sellafield, such as the origins of groundwater salinity, the residence age of it, and its flow pathways. Although there have been a series of models developed at Sellafield (Heathcote *et al,* 1996), most of them were small scale and they were used mainly to deal with superficial fresh water flow. Previous work of modelling remained at the initial level of reproducing the groundwater head, and no models had been calibrated or validated. Groundwater modelling in this thesis is intend to help understand the potential migration of radioactive waste away from the repository zone, and the regional-scale pathway of groundwater flow from the mountain recharge area to the coastal discharge area. Modelling also helps to constrain the regional scale geophysical parameters, e.g. by calibrating the model against measured, in-situ data.

The application of numerical models to regional low permeability rocks is very difficult due to the lack of worldwide experience, scarcity of data, and long prediction horizons. I have constructed a regional 2-D cross section model to represent the regional groundwater flow and heat transport. This cross section starts from the East Irish Sea, goes north-eastwards through Sellafield, and the Lake District Block, ending at the Alston Block. The section is 115 km long and 7.3 km deep. To discretise the region, 3750 nodal points and 7500 triangular elements are used in a finite element approach.

This study was divided into several stages trying to investigate the biases and important controls in the modelling and to reproduce both local and regional groundwater flow systems. In particular, the aim was to reproduce the water head and flow pattern in the BVG where the repository volume might be located. This study also tackled features of water properties, flow patterns associated with streamlines, and heat transportation. In order to minimise the effect of boundary conditions on the calculation, the side boundaries of the model were chosen over 50 km from the repository area. This study focuses on investigating the roles of salinity, permeability and heterogeneity in controlling groundwater flow in West Cumbria. To understand scale effects in previous attempts at Sellafield, a smaller scale local section has been extracted and compared with the regional models. It is important to note that for each model realization the full regional model has been used, even if only the local section has been portrayed in the thesis. Geochemical evaluation of groundwater was made to analyse the indirect evidence of the site's historic evaluation and the long term processes that have led to today's conditions; these help to build confidence for the predictions made into the future. This work includes an evaluation of groundwater chemistry and the development of models for the origin of different groundwaters. The sensitivity test process is used to reduce those uncertainties, assessing both geological and geometrical conditions. During these sensitivity tests, the data measured under in-situ, natural conditions were used to guide the test's reliability.

With the success of reproducing both groundwater head and groundwater flow regimes, identifying uncertainties, a mass transportation model was validated using geochemical and residence age data. The transport model could then be used to predict migration pathways of leachate from the repository site. The result of the study can be summarised as suggesting that radioactive wastes released from the repository site will arrive in the Calder Sandstone aquifer 400m down after 25,000 yr, and some radionuclides will reach the Irish Sea in 50,000 – 80,000 yr.

1 SUMMARY

1.1 Conceptual model

The construction of numerical models is a progressive process. A conceptual model is not trivial, either to define a numerical model, or interpret the data from a hydrogeological investigation. It is the most important and difficult step in modelling. Even a minor misjudgment or wrong presumption will cause a totally wrong calculation result. The difference between my regional model and other worker's local models is that the boundary of my regional model is wider and much more recharge is considered. The area of interest (the repository zone) is a long way from edge effects at my model boundaries. In particular, the low permeability basement and hills area are involved in my regional models, and these are very important to the deep flow systems. There are two sources of salinity, one is from the East Irish Sea Basin Regime. This produces brine waters and the flow is almost static. The other source is from the Hills-Basement Regime, where groundwater flow is very slow due to the low hydraulic conductivity of the Basement. As a result, water-rock interactions may take place, which might increase the amount of total dissolved solids.

1.2 Model development and calibration

The groundwater flow at Sellafield was simulated progressively from a simple three-layer model to a very complicated comprehensive model. During these modelling steps, the modelled water heads in boreholes approach progressively closer to the measured field values, as we develop from the simple model to the comprehensive one (Figure 7-1). This implies that the concept of these models becomes progressively closer to the real system. The first stage of modelling was to use a three-layer model, to test the credibility of assumptions in a conceptual model with respect to head and flow in a most simplified system. The hydraulic properties of the materials were tentatively tested using only groundwater heads measured in deep Borehole 3 at this stage of modelling. The second stage of modelling was to use a Seven-layer Model, incorporating most of the stratigraphy, to investigate lithostratigraphical effects on groundwater flow. The results of the tests were analysed using data from Borehole 3 and Borehole 2, located three kilometers apart. Assessment of those modelled groundwater heads was carried out by plotting heads against depth. The sensitivity tests in this Seven-layer model indicate that the groundwater head is significantly sensitive to changes in hydraulic parameters, which vary from layer to layer or from borehole to borehole even within the same stratigraphy. Among the lithologies, the Calder Sandstone, the BVG, and the Skiddaw Group produce a great deal of response of calculated heads in shallow boreholes caused by the changes of rock permeability at depth. The monitored heads in Borehole 2 and Borehole 3 used in assessment can be matched very well in this Seven-layer Model. The most striking point is that the groundwater head can be successfully reproduced using this regional model. This is especially so for the heads in Borehole 2, in which the heads modelled by others (Heathcote *et al*, 1996) were far below the measured in-situ values. The reason for this might be that the low permeability Skiddaw Slate basement which has previously been neglected was explicitly considered in my regional model. This deep rock unit plays an important part in the regional model and in particular in the deep groundwater flow.

The response of the modelled groundwater heads to the sensitivity tests of hydraulic properties of the rock varied from borehole to borehole. More complexity resulted from introducing more borehole data to match the modelled values. Therefore, data from three deep boreholes were used to test the credibility of the model. They are Borehole 3, Borehole 2, and Borehole 10A. Generally speaking, the more measured borehole head data that was introduced to be matched, the more difficulties were encountered in trying to match them all at the same time. This is because the parameters for the model matching one borehole do not necessarily suit the others. It should be appreciated that all of the heads measured in these boreholes showed a better match between calculated and measured values after introducing the Comprehensive Model, in which all the materials discovered at Sellafield were involved in the model, explicitly including Drift, and Fault Zones. It should also be noted that the best fit parameters are close to the median values of the field measurements of the rocks.

Examination of groundwater flow modelling indicates that the groundwater flow system modelled is consistent with the conceptual model. This suggests that the groundwaters are recharged from precipitation in the eastern hill areas, percolating through the Granite and the BVG, going down and then rising west upwards into the sediments, and finally flowing towards the west coast (Figure 7-3). This still shows that the groundwater in the repository zone is recharged both from the basement and by lateral flow from an eastern boundary. Most of the fresh water goes directly into the superficial aquifer after precipitation, and discharges to the west coast, forming the Coastal Shallow Water Regime (Figure 7-4). There is also shallow, rapid, groundwater flow existing above the brine water regime driven by topography from the coast towards the center of the Irish Sea with the flow rate about 1 m/yr. The brine waters in the East Irish Sea Basin Regime are almost static.

1.3 Modification of the Model

From previous stages of modelling it is suggested that the more complex and well characterised the system being studied is, the better agreement is achieved between model predictions and observations of the system behavior. It is obvious from studying the modelling that an increase in scale and complexity of the system leads to a better fit between the model and the data. This is often with an attendant increase in the quality of characterization of the structure of the system, i.e. the geometry, boundary conditions, as well as the heterogeneity and anisotropy of the materials. Because of the limitation of the computer memory, it is likely that element construction in the regional model is so coarse that numerical dispersion could happen. If this was so, the regional mesh could not reproduce accurately the local groundwater flow system if the mesh constructed is too coarse to represent the geological structures in detail. To reduce these impacts, it is necessary to modify the model both geometrically and conceptually. This modification was achieved by increasing the number of finite elements across each fault zone, and by reforming the size and shape of the finite elements in the rock units. The improvement is very significant in this study (see Figure 7-2) and the modified model can reproduce the measured freshwater head of all three boreholes. In other words, the modified model can adequately represent the real groundwater flow system at Sellafield, both at local size and at regional size.

The regional model clearly reveals the basic features of the regional groundwater flow systems, which have not been adequately studied before. The eastern part of the area, land and hill, is the recharge area; and the upper western area, the East Irish Sea, is the discharge area. The groundwater is recharged from precipitation, percolates into the subsurface, and flows east towards the coast. Most of the water flows superficially. The deeper western area is almost a no-flux area. It should be noted that groundwater flows through the PRZ are recharged laterally from precipitation in the mountain area. This rainfall percolates into the deep subsurface, and takes a long journey across the repository site (Figure 7-3) to the offshore. Based on the results of modelling, the groundwater flow regime can be divided into three parts: the Shallow Water Regime, distributed in the Sandstone Groups on the coast and off shore; the Inland Groundwater Regime, distributed in the eastern land and hill area; and in the deep East Irish Sea Basin under -1.5 km OD, where there is almost no flux except other than convection resulting from the variance of salinity, this is termed the East Irish Sea Basin Regime. The regional modelling also shows that there are two possible sources of salinity, one is the East Irish Sea Basin Regime, from halite bearing rocks. The other is the Inland Groundwater Regime, from the water-rock interaction during the long time and long distance of travel. The variation of salinity was observed and calculated from the field measurements, either from total dissolved solid values for the groundwater samples, or from electrical conductivity data. There might be two sources of salinity. All the differences between groundwater chemical components measured from in-situ samples and acting as natural tracers reveal that the origins of groundwaters are different in different boreholes. The major basinal component is in Borehole 3 at the coastline; the inland component is dominant in Borehole 2 at the PRZ; while a mixture of the components is in Borehole 10A in the middle. This two component mixing phenomenon is well reproduced in this modelling Figure (7-4). The most striking point is that the flow regime derived from groundwater flow modelling agrees well with the independent data from distribution of measured chemical components.

1.4 Comparison of models

Since the results of modelling vary from model to model, it is necessary to find the reasons causing this difference and to build confidence in the modelling. Comparisons can only be made when identical conditions are set. Through the comparison of these models in many respects, such as fresh water head, groundwater contours, stream line contours and groundwater flow field, the main reasons why the results of the regional model are different from the local model are determined. The same results were obtained in my district model as NIREX achieved using their models. In comparing McKeown's (1999) model with my district model, the very high hydraulic conductivity of the BVG obtained from McKeown's work was also reproduced. However, this high value did not match the head in BH10, which was not involved in McKeown's work. The important thing is that although the freshwater head in BH2 can be reproduced in a local model by input of very high hydraulic conductivities for the BVG, these could not reproduce the total local flow system with respect to either flow velocity or flow path (Figure 7-5), and this will inevitably influence the prediction of the safety of the proposed repository site (Figure 7-6). The low permeability rocks at depth take a very important part in both the shallow and the deep underground water flow system, even though flow is always small compared to the higher permeability shallow aquifer systems. However, deep flow should not be neglected in dealing with low permeability rocks. The importance of low permeability rocks in regional deep groundwater flow systems has been proved in this study. The reason why NIREX predictions of fresh water head in their local models were below the measured value (Heathcote *et al*, 1996) is that the recharge from deep low permeability rocks was neglected. The eastern vertical boundary should not be treated as a no-flow boundary in the local models. Not only was the groundwater head affected by restrictions NIREX used on their local model, but also the groundwater flow rate in the BVG around the proposed repository site location was apparently influenced as well. My regional modelling result suggested that the flow rate in the PRZ was about 1.0 m/yr, where the local model as NIREX restricted predicted a 0.1 m/yr flow rate. This will directly affect the prediction of the performance of the repository site.

1.5 Prediction of radionuclide migration

Having an appropriate representation of the velocity field, which has been fully made available through the procedures described in the preceding chapters, we can simulate mass transport. Numerical modelling of radionuclide transport provides an insight into the potential performance of a radioactive waste repository site. The previous numerical modelling of Sellafield was performed by a number of organizations working together (Heathcote et al. 1996), with emphasis on reproducing the groundwater head at the repository site. None of their work was involved in simulating radionuclide transportation. In this present study, the migration of groundwater from recharge areas to the repository site was simulated using OILGEN's mass transport capabilities, and both dynamic dispersion and molecular diffusion are involved. Transport calculations in repository performance assessments are based directly or indirectly on the groundwater flow characteristics. There are still uncertainties in the basis of transport modelling. It is critical to choose suitable parameters to feed into the model of mass transport in groundwater. One approach to the problem is to use hydrogeochemical data to determine effective transport parameters directly.

In general, all transport models are based on the principle of conservation of mass. Advection and dispersion are regarded as being the major phenomena transporting radionuclides leaching from a nuclear waste repository. The flow-rate of water in the ground is calculated by Darcy's law, and the transport of solute by the so-called advection-dispersion equation. The advection-dispersion transport equation is more difficult to solve numerically than the flow equation. The advantage of the random walk method, particularly, is that it performs well for large Peclet numbers. The other advantage of the random walk method is that it conserves mass, even if the flow field is not computed with high precision, and may not require the solution of large systems of equations. In the prediction of radioactive waste migration, what we want to understand is the first arrival of the radionuclides. To this end, the particle tracking method is the most effective way to help us to investigate it.

The stable isotopes ($\delta\,^{2}$H and $\delta\,^{18}$O) for groundwater samples in the basement rocks of the repository site have a meteoric signature. The stable isotopic signatures and recharge temperatures derived from noble gas abundances in the groundwater samples indicate that recharge conditions for groundwaters in the BVG of the PRZ were colder than recharge in the overlying sandstones. Both stable isotope composition and inert gas contents depend on climatic conditions at the time of recharge (infiltration), and all these indicate that the recharge of the basement rocks in the PRZ was under colder climatic conditions before the last glacial period ended 10,000 years ago. The groundwater age can also be estimated by investigating groundwater travel times predicted using a groundwater flow model (Toth and Sheng, 1996). This modelling of groundwater reveals that the groundwater in the repository site is recharged from precipitation in the mountain area, and that the groundwater residence time at the proposed repository site is at least 0.14 million years. That is coincident with the measured geochemical data from ^{14}C, ^{3}He, $^{36}Cl/Cl$, which indicate groundwater at the PRZ is older than 30,000 years and younger than 1.5 million years.

Site characterization is associated with several sources of potential errors and uncertainties. Many of the parameters used in the site evaluation, e.g. hydraulic conductivity and dispersivity, cannot be directly measured but need to be estimated indirectly using interpretation models. One approach to the problem is to use hydrogeochemical data as long lived natural tracers to determine effective average transport parameters directly. Since the location of surface recharge of the groundwater into the repository site has been determined, a more effective method of determining average transport parameters directly is by fitting model predictions to measured data of groundwater age. Both hydraulic parameters of the rocks and flow lines of groundwaters can be evaluated using measured chemical data, and the model prediction results agree with the independent results of sensitivity testing via the data of groundwater. It is found that the groundwater travel time obtained by means of stream line isochrons is about 150,000 years at the repository site, 10,000 years older than the dispersion method, which means that the error might be about 7% using the stream line isochron method.

With those uncertainties being fixed, it is possible to make predictions into the future potential. The radionuclide transport from the repository site can be considered in three stages (Figure5-7): Firstly, they would migrate in the BVG, then pass into Sherwood Sandstone Group after 3,000 years; secondly, after about 25,000 years, they arrive at the aquifer of the Calder Sandstone. At last, some of them will reach the sea water of East Irish Sea in about 50,000 years. Most of the radionuclides released from the disposal site will be transported west towards to the offshore under the seabed of East Irish Sea. Consequently, the return time for the first arrival of radionuclides from the disposal site back to the surface is between 50,000 years and 80,000 years.

2 CONCLUSION

From the analysis and investigation of hydrogeochemical data in deep boreholes at Sellafield, the predicted flow field is coincident both with measured data and the conceptual model. The characteristics of groundwater flow have been linked with the successful reproduction of a groundwater flow field. Therefore the predictions of radionuclide migration using this calibrated mass transport model should be reasonable. Through the comparison of these models, the following conclusions can be drawn:

— The Regional Model simulates the groundwater system better than the local models at Sellafield, in reproducing both the measured groundwater head in boreholes and the recharge area.

— There are many differences between modelling results from the Regional Model and those of the District Model. These differences can be displayed through the head pattern, water flow velocity and water flux.

— There are general similarities among previously published local models and the district model. The same results can be obtained if the same conditions are set.

— There are no obvious scale effects in the Regional Model, the best fit parameters in the regional model are close to the field median permeability of the rocks measured in-situ.

— The reason why the fresh water head obtained from the local model was below the measured value, is that the recharge from the low permeability rocks at depths greater than 2 km has been neglected. The eastern vertical boundary should not be treated as a no-flow boundary in the local models.

— The groundwater head obtained from local models in BH2 can be raised by setting higher hydraulic conductivity value in the BVG, but this cannot explain the head in BH10. Consequently, the flow pattern obtained from such models cannot accurately represent the actual system.

— The low permeability rocks play a very important part in the deep underground water flow system, even though these flows are smaller than these in shallow aquifers. Hence, small flows in deeply buried low permeability rocks should not be neglected in modelling groundwater flow.

— The groundwater head was affected by the restrictions of the local model. Consequently the groundwater flow rate in the BVG where the proposed repository site is located was influenced as well. The regional modelling results suggest that the flow rate in the PRZ is about 1.0 m/yr, where the district model predicts much slower flows of 0.1 m/yr.

From the analysis and investigation of hydrogeochemical data in deep boreholes at Sellafield, the predicted flow field is coincident both with measured data of heads and the geochemical composition and the conceptual model. The characteristics of groundwater flow have been linked with the successful reproduction of a groundwater flow field. Therefore the predictions of radionuclide migration using this calibrated mass transport model should be reasonable. Accordingly, these conclusions can be drawn:

— The flow path of groundwater was reproduced using the models. The modelling produced two distinct flow regimes, and these coincide with the two different measured hydrochemical components. The groundwater flow path into the repository site originates from precipitation in mountain areas 16 km to the east. The flow path from the repository extends to reach the surface in the Sherwood Sandstone Group 4 km west.

— Based on groundwater flux and its route, the groundwater flow system can be divided into: 1) a Shallow Flow Region that has a short travel distance and a large flux, 2) an Inland Flow Region with a long distance but small flux, and 3) the Irish Sea Basin Region which has little flux.

— From this modelling, there are two sources of salinity in groundwater at Sellafield, one is the Inland Flow Region resulting from water and rock interaction to the east; and the other is the Irish Sea Basin Region resulting from the dissolution of halite to the west. These correspond with measured geochemical data.

— The groundwater residence time modelled at the proposed repository site is at least 0.14 million years. The deeper groundwaters have older ages. These correspond with geochemical data.

— Isotopic measurements of groundwater residence age show that groundwater in the PRZ is older than 30,000 thousand years, and younger than 1,500, 000 years. Results of modelling suggest that the residence age of groundwater at the repository site is at least 140,000 years. This is quite well in agreement with the stable isotope data ($\delta\ ^{2}H$ and $\delta\ ^{18}O$) for groundwater samples in basement rocks of the repository site, which shows that the groundwater of the basement rocks of the PRZ was recharged into the flow system under colder climatic conditions before the last glacial period that ended 10,000 years ago.

— Both the hydraulic parameters of the rocks and the flow lines of groundwaters can also be calibrated using chemical data and isotopic data measured from deep borehole samples, which agree with the results of sensitivity tests via the groundwater head discussed in Chapter 4. Validation of mass transport models via dating the groundwater indicates that the hydraulic conductivity of the BVG also controls the residence time of groundwater at the repository site. It is suggested that the hydraulic conductivity of the BVG should be 0.12m/yr. This is less than the 1.22 m/yr proposed by McKeown (1997).

— It is found that the groundwater travel time obtained by means of stream line isochron is about 150,000 years residence age at the repository site, 10,000 years older than the dispersion method, which means that the error is about 7% using the streamline isochron method.

— Predictions from this modelling suggest that the radionuclides released from the repository site will migrate underneath the East Irish Sea. Only a minority of them will reach the seabed. Return time for radionuclides released from the PRZ site to surface of the sea bed of the East Irish Sea, is between 50,000 and 80,000 years, 3 km west from the PRZ. But these radionuclides will arrive at the Calder Sandstone aquifer at a depth of 400 m within about 25,000 years, 2 km west from the PRZ.

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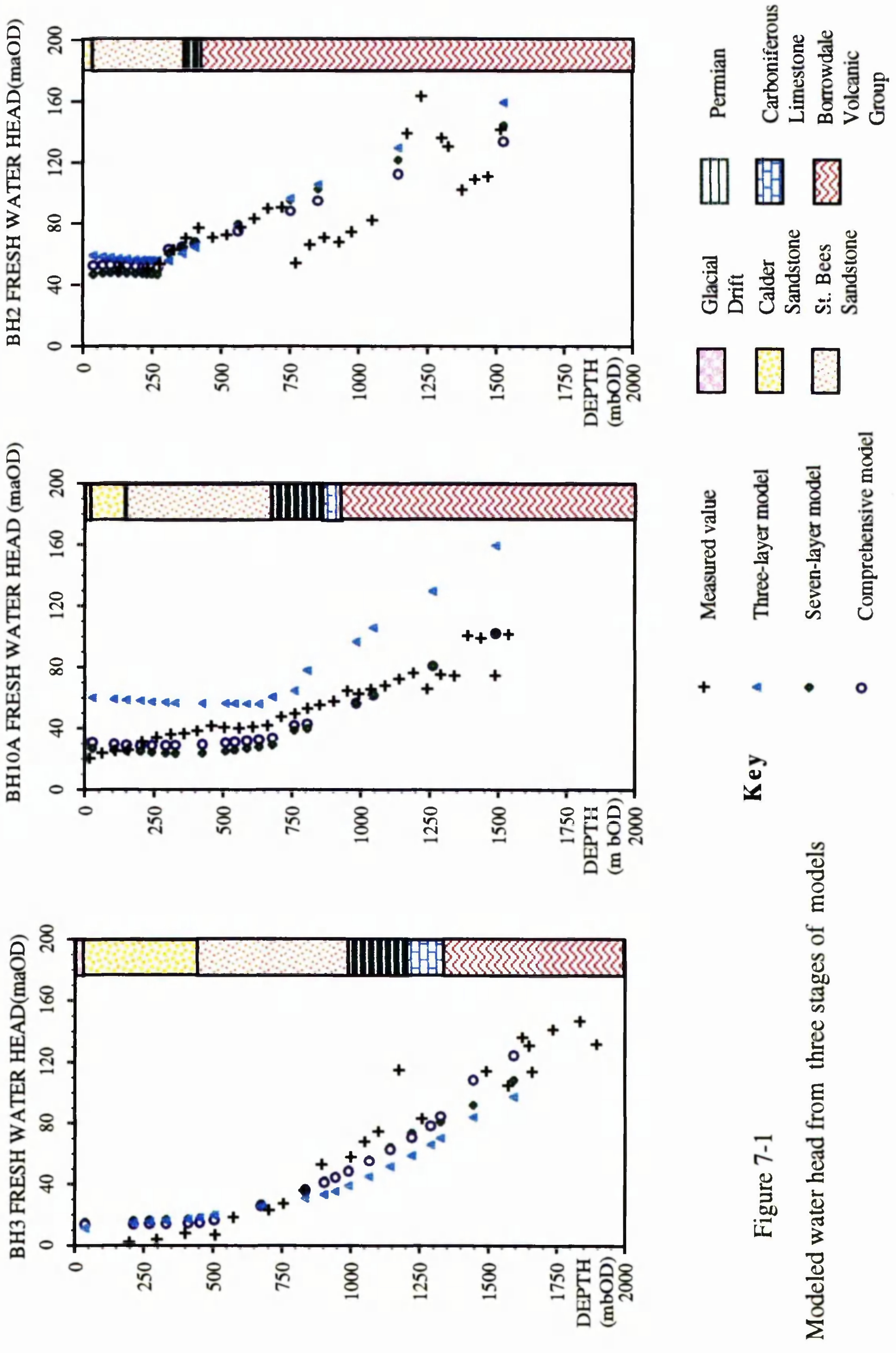


Figure 7-1

Modeled water head from three stages of models

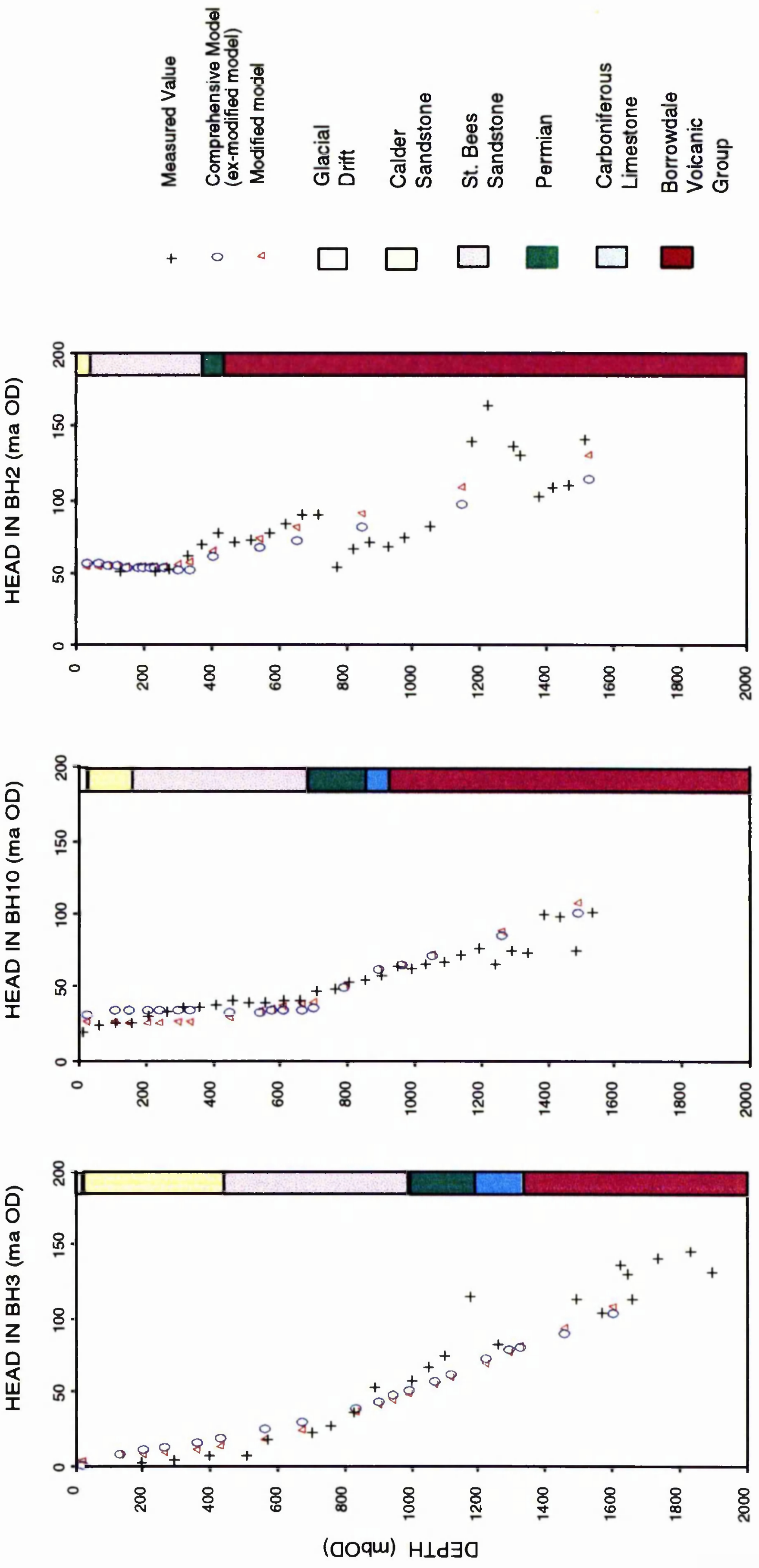


Figure 7-2 The final best fit modelled head

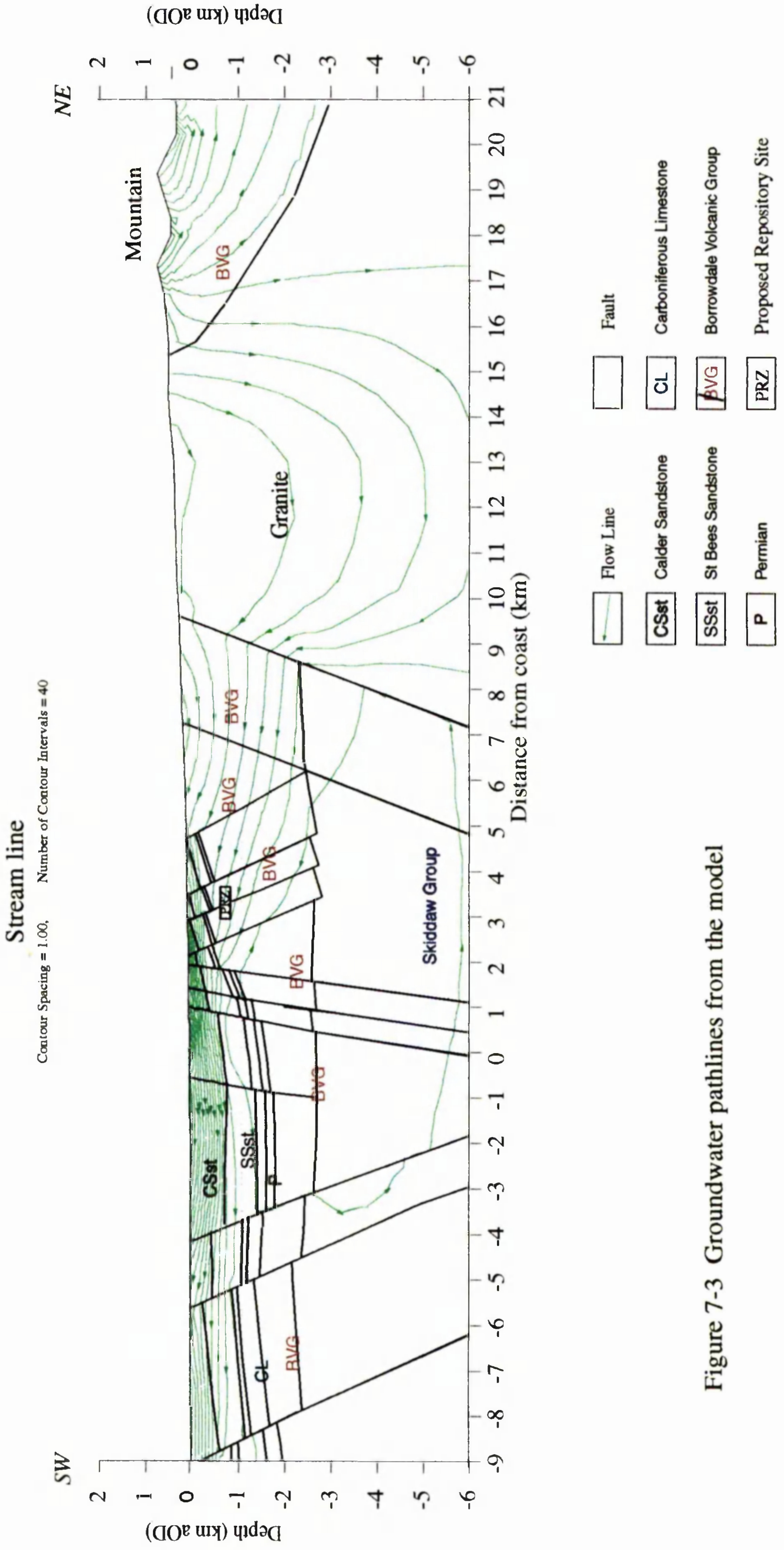


Figure 7-3 Groundwater pathlines from the model

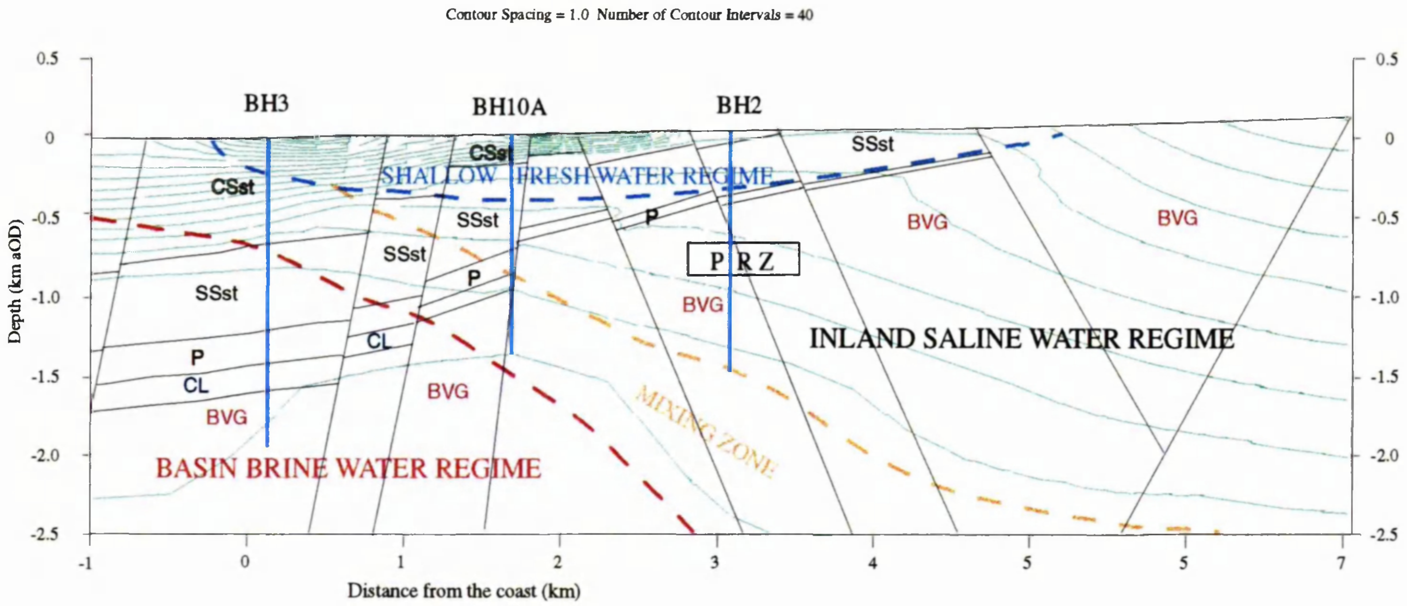
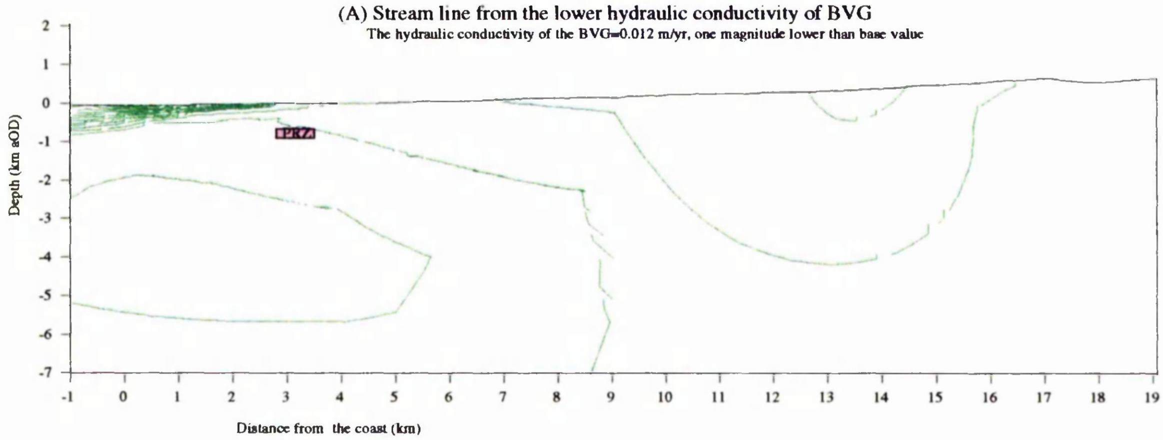
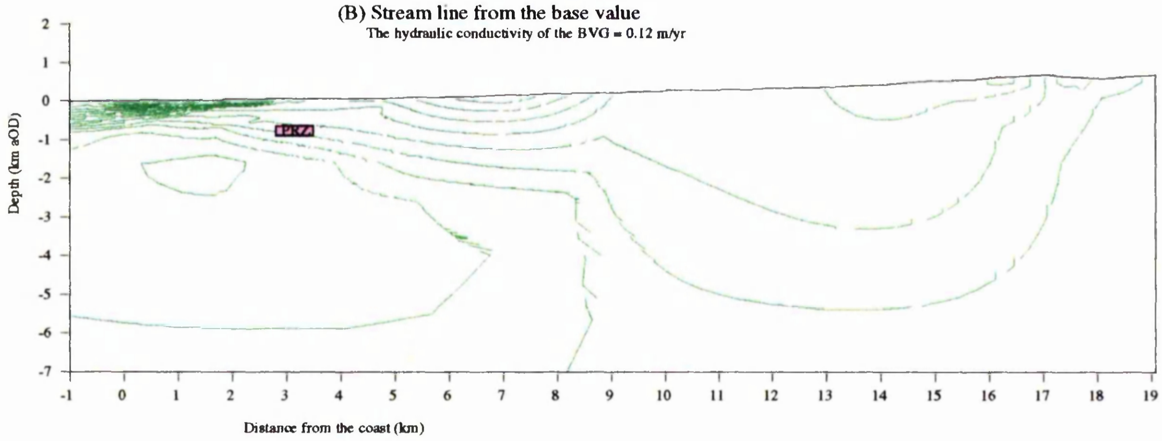


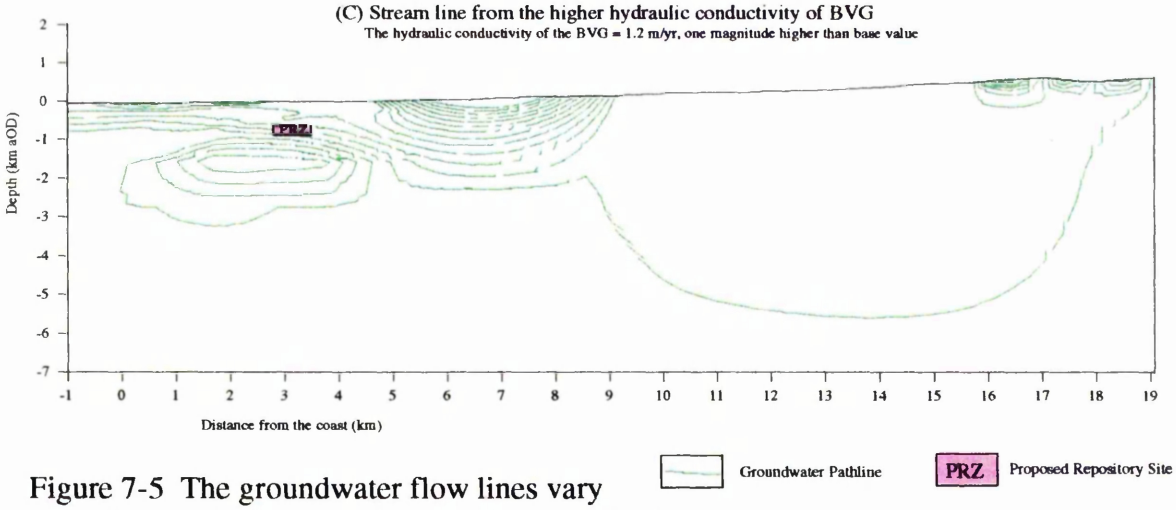
Figure 7-4 Groundwater Flow System Division Based on Flow Line


(A) Stream line from the lower hydraulic conductivity of BVG

The hydraulic conductivity of the BVG=0.012 m/yr, one magnitude lower than base value


(B) Stream line from the base value

The hydraulic conductivity of the BVG = 0.12 m/yr


(C) Stream line from the higher hydraulic conductivity of BVG

The hydraulic conductivity of the BVG = 1.2 m/yr, one magnitude higher than base value

Figure 7-5 The groundwater flow lines vary with different hydraulic conductivities of the BVG

(A) and (C) shows the flow pathline will not reach the PRZ if the hydraulic conductivity of the BVG is either 0.012 m/yr (lower than the base value), or 1.2 m/yr (higher than the base value).

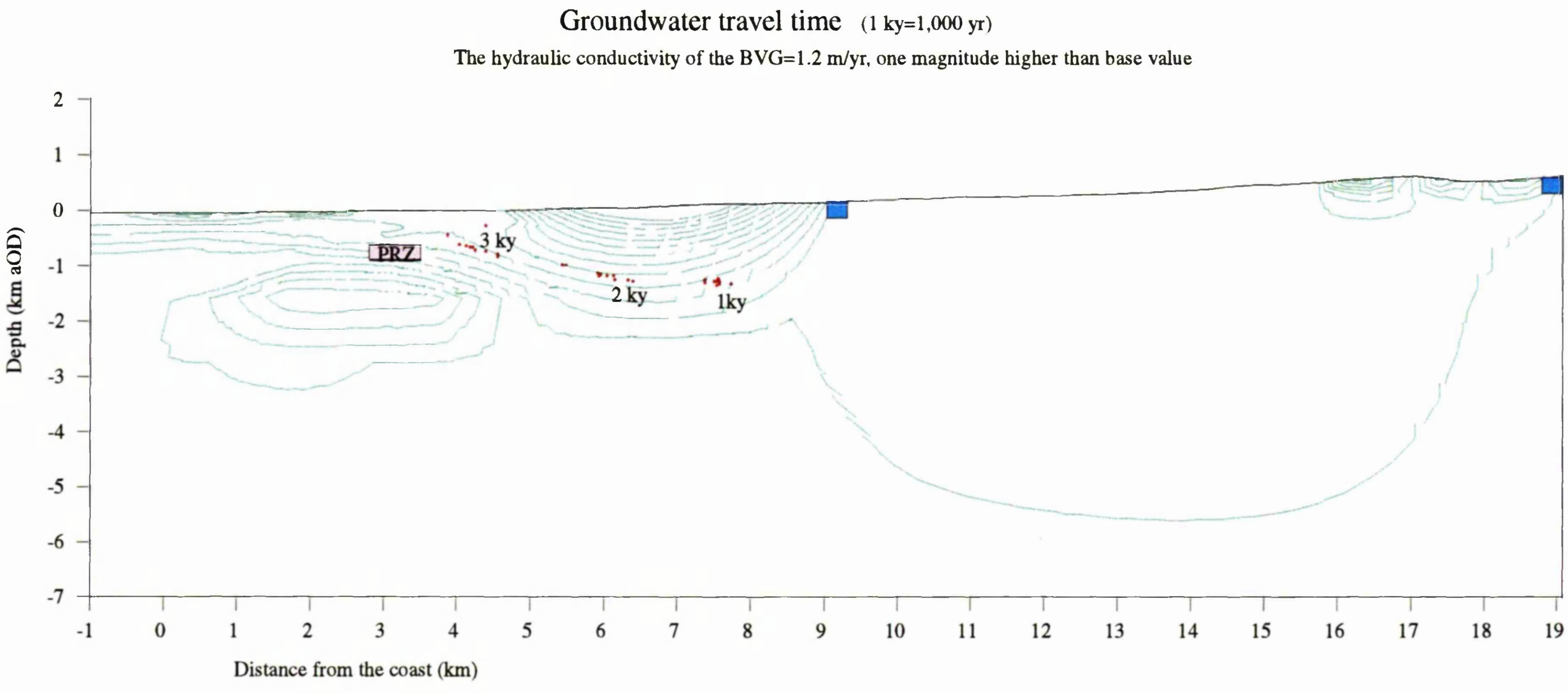


Figure 7-6 Groundwater travel time predicted from the model

The time of groundwater travel will be very short, only a few thousand years,
as a result of higher hydraulic conductivity of the BVG,
if the hydraulic conductivity of the BVG=1.2 m/yr, one magnitude higher than base value

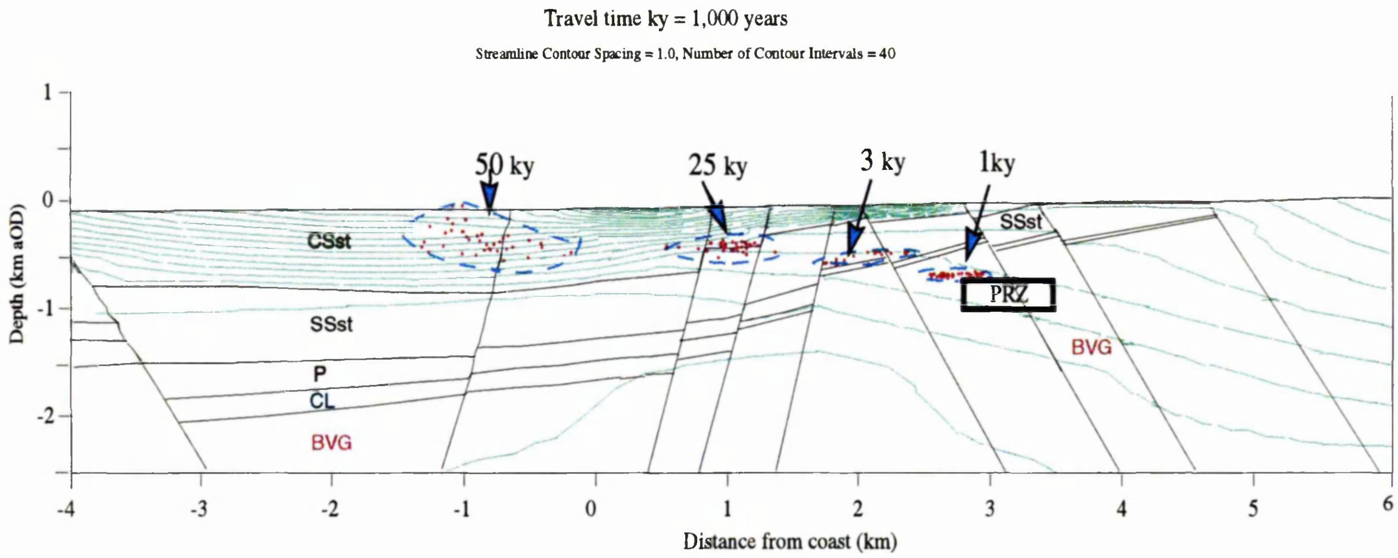


Figure 7-7 Prediction of Radionuclides Migration

It shows that the radionuclides will go into the Calder Sandstone by 3 thousand years, reach to the sea bed about 50,000 years