R-07-03

Sampling of surface water and shallow groundwater at Laxemar

Possible indicators for interaction between deep groundwater and water in contact with the biosphere

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January 2007

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Keywords: Surface water, Shallow groundwater, Deep groundwater, Mixing, Dilution, Modelling, Biosphere, Groundwater sampling.

Abstract

The possibility of an upward flow of saline groundwater with long residence time and its mixing with young recharge waters has been studied in the Laxemar area, situated on the main land north/northwest of the Äspö underground Hard Rock Laboratory. The knowledge of these near surface processes and transport pathways is essential in order to understand the interaction between recharge and discharge patterns of the groundwater and the possible effect from a faulty repository on the biosphere. Hydrogeological modelling in the literature suggests a major out flow regime along the Baltic coast and therefore, possible traces of deeper saline groundwaters could be expected. A total of 108 samples collected from surface, shallow and deep groundwaters from lakes, ditches, quarries, and wells have been analysed together with samples from the Baltic Sea.

The project was challenging due to sampling (difficult to identify representative sampling locations), analytical (low concentrations are associated with high uncertainties) and modelling difficulties (strong dilution gives weak indications in analyses and hence in the models; complex mixing patterns due to several end-member mixing; and reactions which can alter the signature of the waters). The results indicated that the obtained Cl content which is known to be a water conservative tracer had a similar content at the depth of 500 m (repository depth) as at 1 m depth, in addition natural elements such as e.g. Rb and Cs correlated with Cl. By just correlating element concentrations with Cl measurements erroneous impressions of water conservative transport may occur.

No conclusive proofs of transport of deep water up to the surface have been found in this study, but there is nothing that contradicts this assumption either. The waters sampled are between meteoric-sea water and meteoric-deep water. The model calculations show that if a transport takes place this is a slow process in the orders of thousands of years and the dilution is large. The modelling indicated that a small fraction (around 2%) of the measured values at the surface was derived from the 500 m depth. In addition water rock interaction processes along the flow paths retards the transport and it makes also the tracing of deep influences difficult. The same pattern occurred despite changing both the reference waters in the modelling and the physical extension of the modelled area (e.g. from 50 m down to 1,000 m). It is concluded from this study that Cl, Ca, SO_4, Rb, Cs and Th can be useful tracers for the transport processes from the repository level to the biosphere but only a minor fraction of their content in the surface waters may be from the repository level. Element content or a ratio between elements alone cannot be used to indicate the deep origin of groundwaters without compensating for possible sources along the flow path. A mixing or transport model for the site can be used for this compensation.

Contents

1 Introduction

In case of a canister failure radionuclides can be transported from the final repository up to the biosphere. Hence the understanding of the near surface processes and transport pathways are essential in order to model such scenarios. Research results /Maitre et al. 1999/ have shown that root systems can extend to a depth of 10 m dependent of the physical conditions and deeper than previously thought (1 m). The interaction between the biosphere and groundwater is also more extensive than previously believed. The aim of this project is to increase the understanding of the interaction between deep groundwater, shallow groundwater and the biosphere (Figure 1-1) in the region close to the Äspö Hard Rock Laboratory. The major aim of the project is therefore to trace possible indications of deep water in contact with the shallow and surface water.

In the Äspö and Laxemar area the deep groundwater is characterised by saline water with high TDS (total dissolved solutes) shown for example in analyses from groundwater in borehole KLX02 /Laaksoharju and Wallin 1997/. In contrast shallow groundwater is characterised by low TDS (with typical rainwater characteristics) and with a short residence time in the ground. Hydrogeological modelling of the Äspö and Laxemar area /Svensson 1997/ suggests a possibility of upward flowing deep saline groundwater in the discharge areas along the Baltic shore line (cf. Figure 2-1,). The present investigation was initiated to trace possible deep upward flowing groundwater by sampling shallow water from wells, streams, lakes and from soil tubes at the shoreline. It was thought that since the deep groundwater has a distinctive signature shown in the major components and stable isotopes, this signature might be traceable in shallow groundwater systems as well.

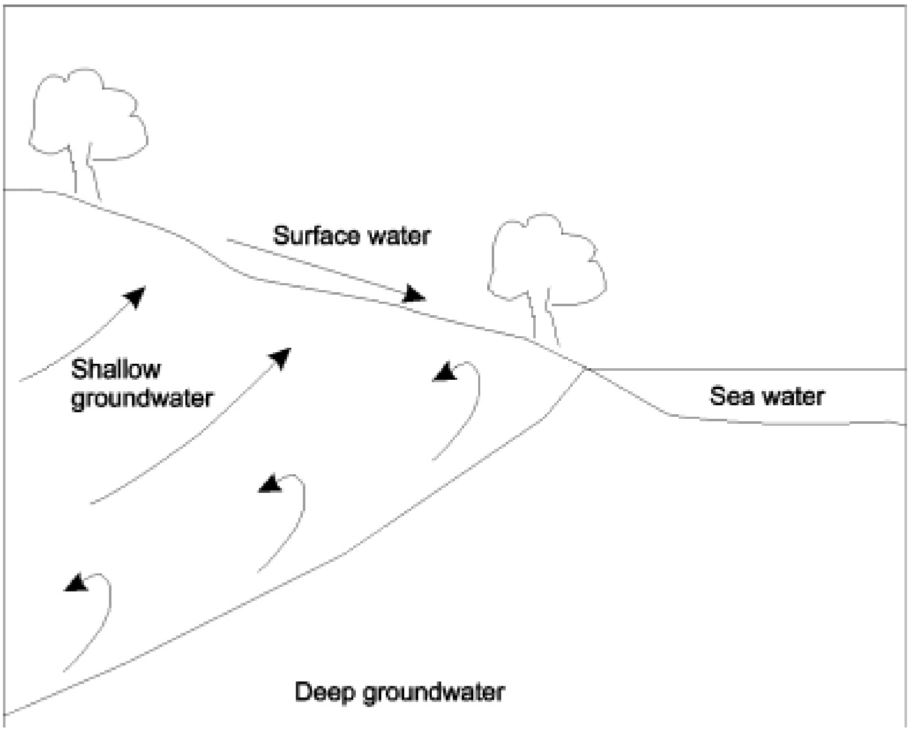


__Figure 1-1.__ Schematic picture showing the possible interaction between deep groundwaters, shallow groundwater and the biosphere. Regional hydrogelogical forces together with annual changes in the groundwater table and fluctuating sea levels can act like a pump which may help the deep groundwater to mix with shallow groundwater, which is then transported, upwards where it may come in contact with the biosphere.

2 Topography, geology and hydrogeology of the site

The area of sampling is within LMV map sheets Vimmerby 6G SO and Kråkelund 6H SV. The topography of the sampled area reaches from sea level to about 30 m above sea level. The mainland rises towards the west. The isostatic land rise is around 1–2 mm/yr in the area /Björck and Svensson 1992/. The highest post-glacial shoreline in the area is situated about 100 m above present sea level in the Oskarshamn area /Svensson 1991/. The landscape is characterised by exposed bedrock on heights, washed till along the slopes and clay/organic soils in the topographical depressions.

The bedrock is mainly of 1,800 Ma old TIB granitoids (Transscandinavian Igneous Belt) except for the younger (c. 1,380 Ma) Götemar granite outcropping in the northwestern part of the studied area /Wikman and Kornfält 1995/. The washed till is rather rich in boulders. Clay fills out larger depressions between the rock heights and is probably mostly of glacial origin. An esker runs through the area from NNW (along the western shore of Lake Götemar) to SSE (towards Ekerum, through Gässhult and Sandsböla). The flat rocks along the southern strand of Kärrsvik are rich in striae in the S140W direction, approximately the same direction as the esker. These two features give an approximate direction of the former continental ice movement in the area.

The results from the hydrodynamic modelling of the area by /Svensson 1997/ shows the groundwater vertical flow at 30 m and 500 m depth for the sampled area (Figure 2-1). Red colour is upward flow and blue is downward flow. The modelling shows that there is a potential for upward flow in the north part of the modelled area shown in green.

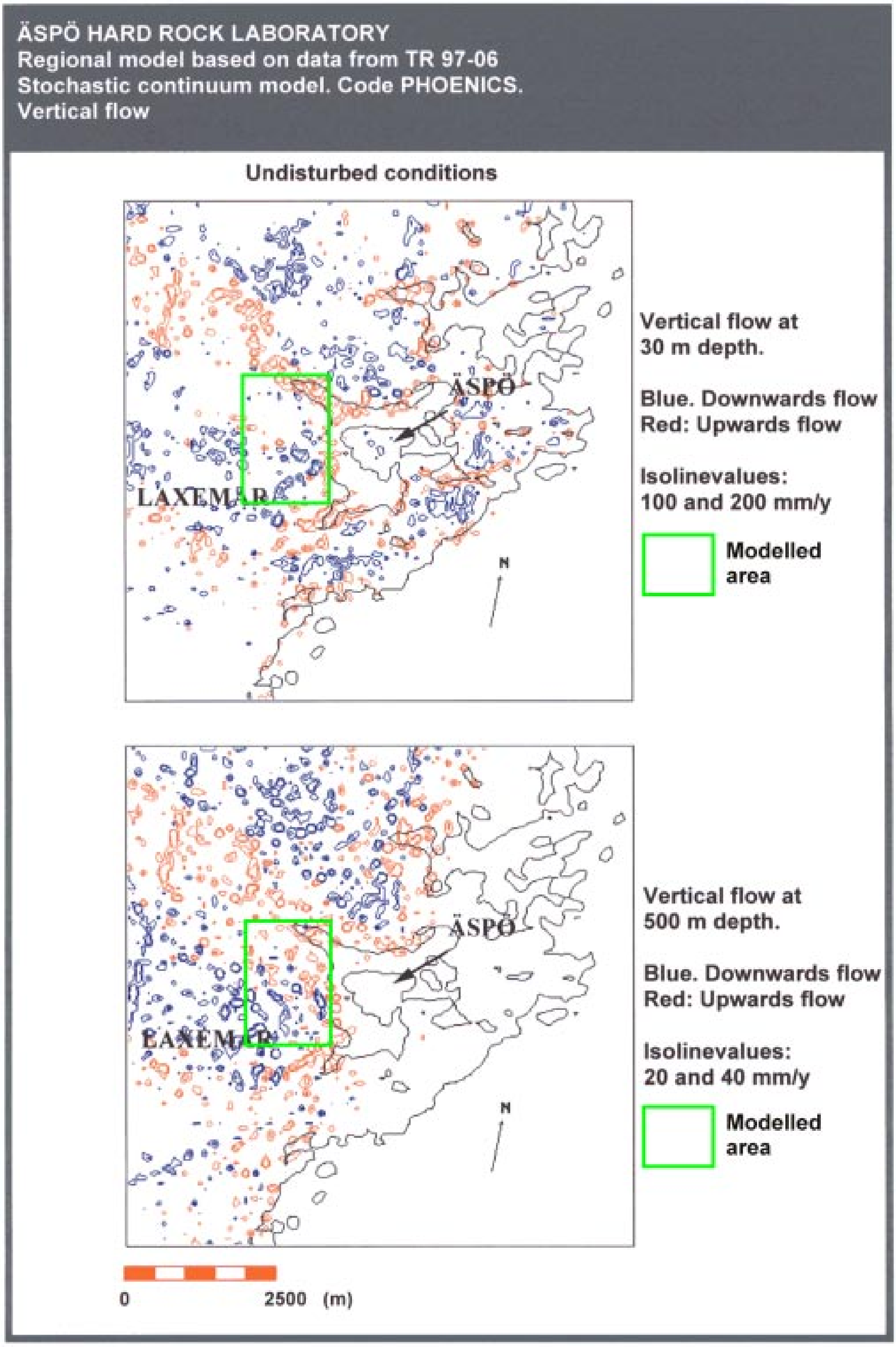


Figure 2-1. *Groundwater vertical flow at 30 m and 500 m depth based on hydrodynamic modelling by /Svensson 1997/. Red = upward flow, blue = downward flow. The area investigated and modelled for this project is within the green square.*

3 Sampling and analyses

For this project three different data sets were used:

Data set A: Contains a total of 45 surface and shallow samples collected in 1998. The samples are collected from ditches, one lake, one open stone quarry, one gravel pit, four points in the Baltic Sea, six wells and eight percussion wells (HLX01 to HLX08) at Laxemar were sampled. The surface and seawater were collected directly into bottles. The percussion wells were sampled with a standard check valve sampler at a depth of 19 to 20 m below ground surface (HLX01 to HLX07) except for HLX08 which was sampled at a depth of 6 to 7 m below ground surface. See Figure 3-1 for sampling locations.

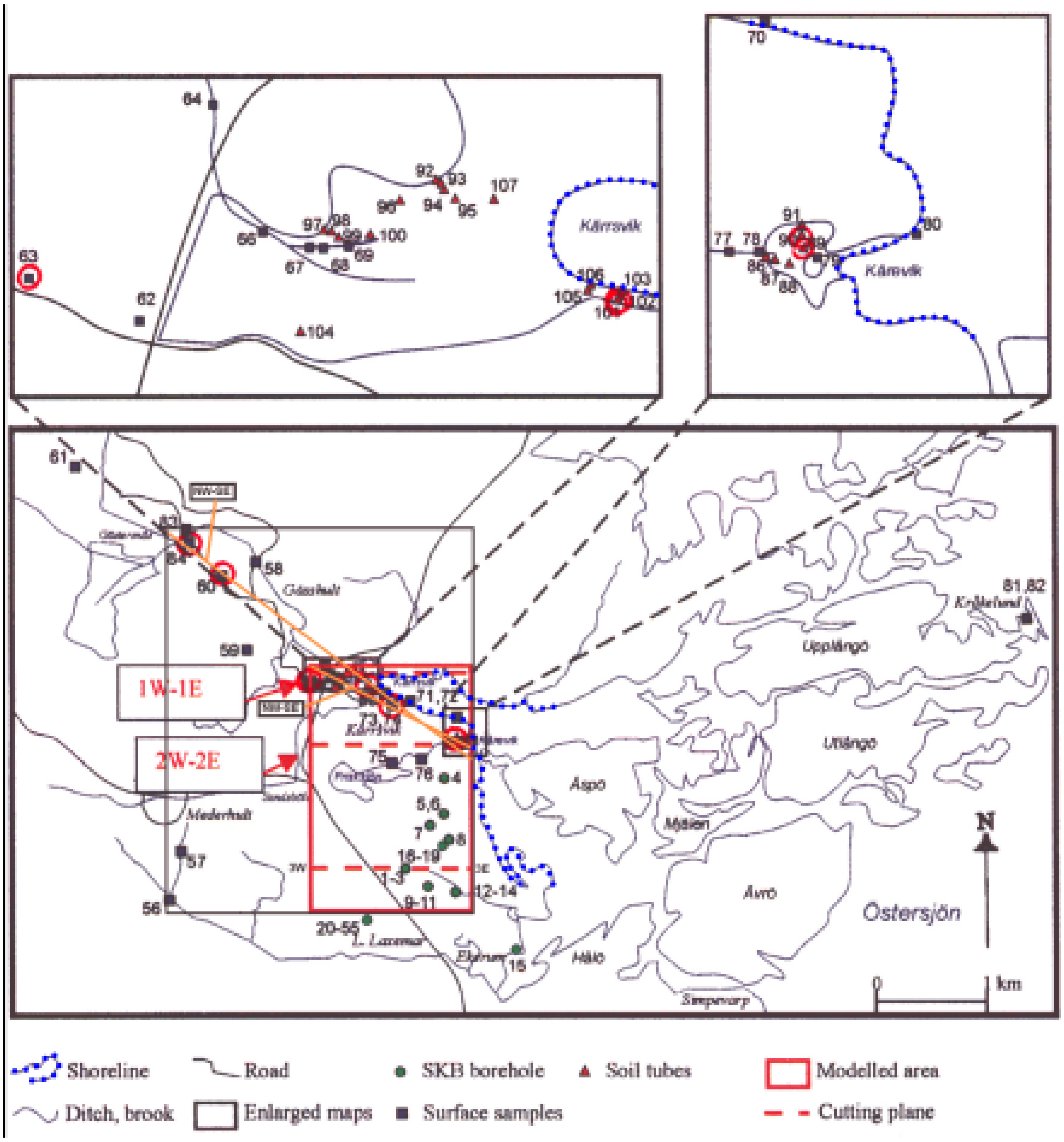


Figure 3-1. Map showing the sampling locations at the site. The following models are represented: the red square shows the modelled area for the superficial box (–56 m depth) and the deep box (–500 m depth) and the black square shows the modelled area for the enlarged box in the NE-SE direction. The profiles 1W-1E, 2W-2E, 3W-3E, and the 2 transects NW-SE (in yellow) represent cutting planes used in the modelling in Figures 6-1 to 6-21. The blue dotted line indicates the shoreline between the Laxemar mainland and the Baltic sea.

Parameters analysed were temperature, pH, conductivity, major components and stable isotopes together with $\delta^{34}S$ in the dissolved sulphate for boreholes HLX01, HLX03, HLX04 and HLX08. The results of the major component analysis are listed in Appendix 1. The analyses followed the SKB standard procedures concerning the analytical methods, detection limits and measurement uncertainties as discussed in /Säfvestad et al. 2000/. The $\delta^{34}S$ analyses were carried out according to the procedure described by Wallin and Peterman (paper #12 in /Laaksoharju and Wallin 1997/).

Data set B: Contains samples collected from 22 standard soil tubes (PEH-tubes) during 1999 which were installed in profiles in the soil close to the shoreline (see Figure 3-2) of the bays Kärrsvik and Kårevik at Laxemar (see Figure 3-1 for sampling locations). The tubes were of a length of 1–5 m and the lower 1 m consists of a filter tube. Fixed groundwater samplers were installed in the tubes to avoid contamination during sampling. The samplers are PEH tubes, have a inner diameter of 2 cm and have a length of 1–5 m (the length of the soil tube). A ball valve was attached to the bottom of the sampler and the top of the sampler is open (see Figure 3-3). To pump water the samplers were lifted up and down manually. The water was poured from the top of the sampler into the sampling bottles. Baltic Sea surface samples from two near shore locations and one ditch (surface water) were also sampled as reference waters. The tubes were emptied and after one week of stabilisation the groundwater was sampled and analysed following the SKB classification no:5 (major components, trace elements and isotopes δO^{18}, δH^2 and H^3). The trace elements are reported in Appendix 2. Water for trace elements analyses were filtered and acidified during sampling. Major components were filtrated and acidified at the Äspö laboratory approximately 2 hours after sampling.

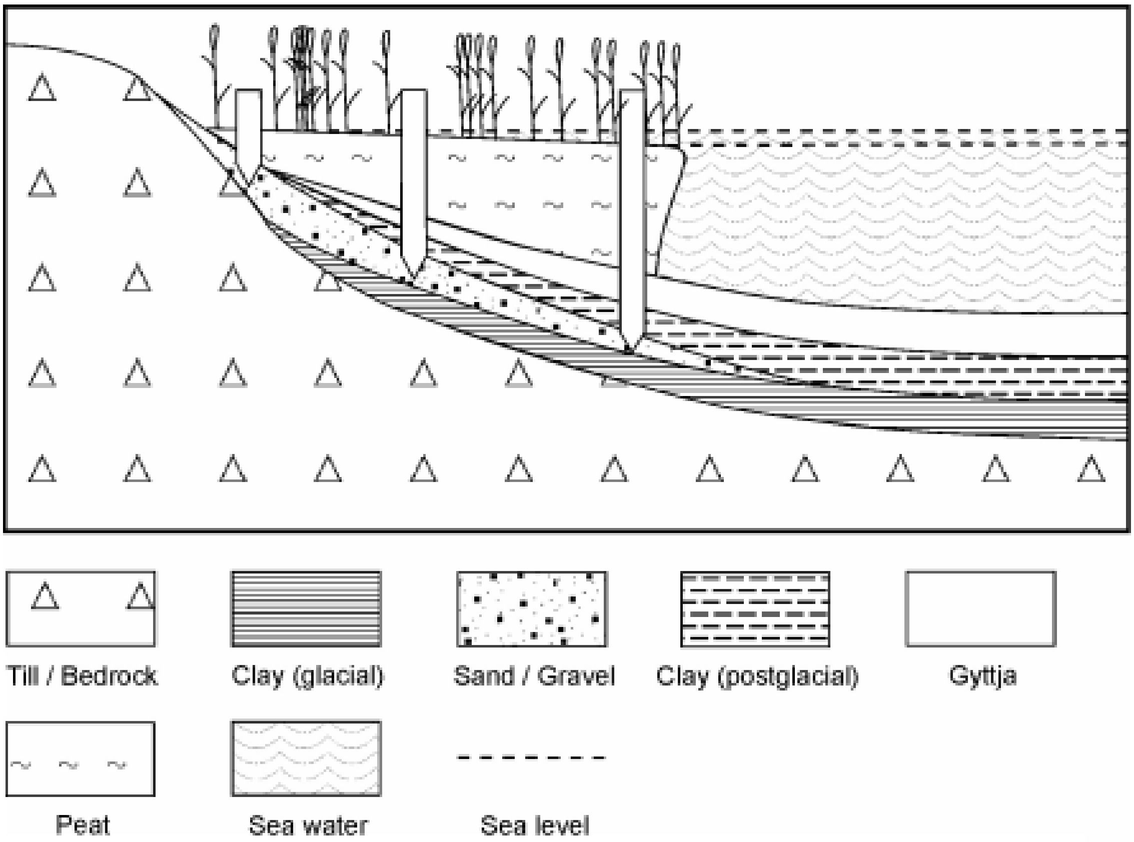


Figure 3-2. Standard soil tubes (PEH-tubes) were installed in profiles in the soil close to the shoreline of the bays Kärrsvik and Kårevik at Laxemar (see Figure 3-1 for sampling locations). The tubes were of a length of 1–5 m and the lower 1 m consists of a filter tube.

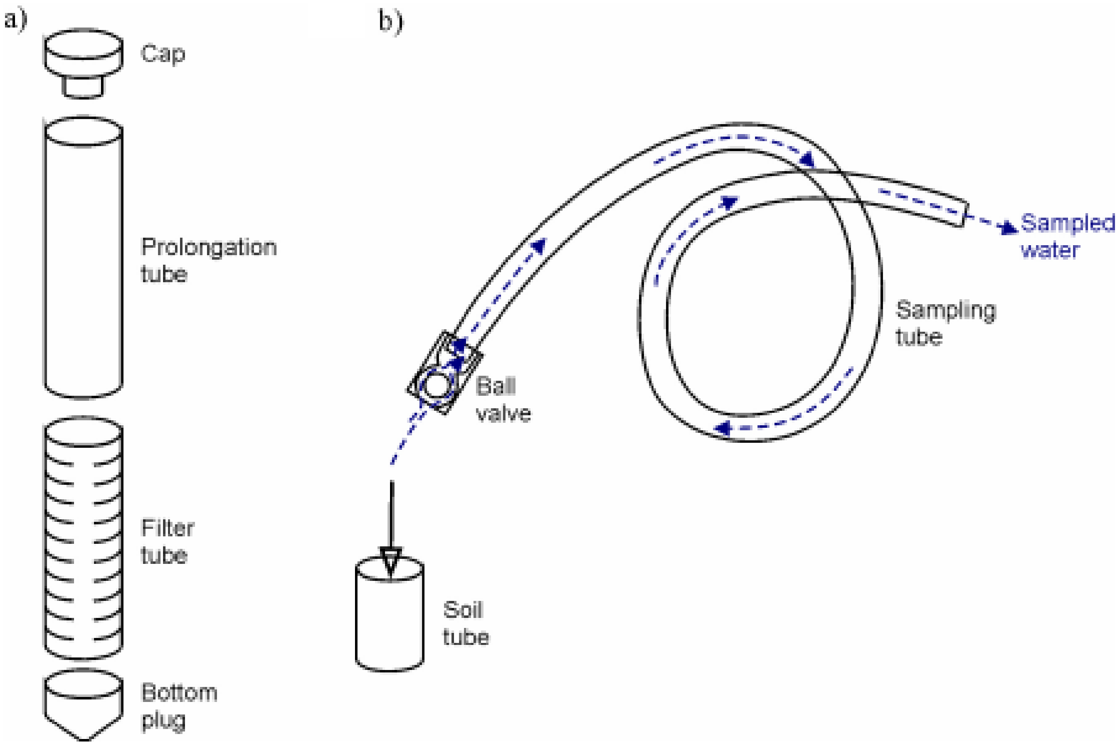


Figure 3-3. *a) The soil tubes were of a length of 1–5 m and the lower 1 m consists of a filter tube. b) Fixed groundwater samplers were installed in the soil tubes to avoid contamination during sampling. A ball valve was attached to the bottom of the sampler and the top of the sampler is open. For sampling the sampler was lifted up and down manually.*

Data set C: The total data set C used in this report contains data set A and B together with 40 samples from deep boreholes (1,000–1,700 m) in combination with precipitation samples. A total of 108 samples have been modelled in this work. The analytical data have been extracted from the SKB database SICADA and are listed in Appendix 1 and 2. Appendix 1 lists major components, stable isotopes and mixing proportions and the deviation from the mixing calculations. For orientation a PCA-plot (Principal Component Analysis – plot) shows the observations as table row numbers. The values are represented graphically as a multi-plot where the variables are plotted against each other in a series of scatter plots. Appendix 2 lists all the observations containing trace elements and multi-plots show the degree of correlation between the analysed elements. Appendix 3 contains more detailed correlations between some trace elements (Th, Rb and Cs) with Cl, operational age and deep saline mixing proportions. The Appendix 4 shows a new M3 calculation where the deep saline end member (no. 17 in Appendix 1) was replaced by the very deep saline end member (no. 41 in Appendix 1). The Appendix 5 shows a test where the elevation and the distance from the sampling point to the sea was included in the PCA. In Appendix 6 the visualisation of the extended profile towards NW (Enlarged box) and the extended box towards the depth of 1,000 m (Very deep box) are presented.

4 Interpretation of the analytical results

The major findings from evaluating the analytical data by means of scatter plots such as the multi-plots in Appendix 1 and 2 are summarised below.

The Ion Charge Balance (ICB) is not satisfying in all surface and shallow samples which may indicate analytical problems for some of these samples /Säfvestad et al. 2,000/. The large negative deviation in ICB for samples HLX01 and HLX03 (ICB around –25%) is suggested to be due to error in bicarbonate content. However, despite a possible overestimate of the HCO_3 content and after correcting the values to ICB O, it is obvious that the HCO_3 content in these samples are very high.

At first the meteoric recharge is the dominating water component in the surface and shallow water. General low salinities (maximum 53 mg/l) together with relatively low $\delta^{18}O$ values support this conclusion. Two samples, no. 64 (259 mg/l, Cl) and 84 (493 mg/l, Cl), have elevated contents of chloride. Both are sampled from drilled wells. No. 64 is situated rather close to the Baltic Sea while no. 84 is situated further away (Figure 3-1). A mixing of marine water is not supported by the $\delta^{18}O$ values in these waters (–10.6 and –10.5‰). In addition the Mg content is low and the Na/Ca ratio is between 5 and 9 compared with > 20 for marine waters. The plot of Cl versus SO_4^{2-} show that the Baltic Sea samples have Cl/SO_4^{2-} ratios around 8 whereas the fresh waters show large variations in Cl/SO_4^{2-} ratios, from 3 to 0.2. This indicates that, for example sea spray are subordinate. Instead leaching of marine sediments may cause fractionation of Cl compared with SO_4^{2-} as Cl is more easily leached than sulphate. Another possibility is the influence of deeper water since sample 84 is located in a discharge area at a depth of 35 m. The M3 mixing modelling in Appendix 1 indicated that the sample no 84 had a marine input of 11% and a deep water input of 24% sample no. 64 was under the detection limit (< 10%) for these water types. A meteoric and Baltic Sea marine component is present in the soil tube samples collected at the interface between land and Sea.

Calcite dissolution together with addition of soil CO_2 is believed to be responsible for the linear relationship between Ca and bicarbonate observed in most of the surface and shallow waters. This is similar to the findings at earlier studies in the Äspö area /Wallin et al. 1995, Tullborg and Gustafsson 1999/. However, biogenic activity is explained to be responsible for the elevated bicarbonate readings observed in some of the shallow water (wells). This is also supported by the low Ca values in these waters.

The $\delta^{18}O$ values can be regarded as a relative indicator of residence time in the ground for sampled water. Waters with high $\delta^{18}O$ value (precipitation from spring and early summer) have a short residence time e.g. the Frisksjön drainage ($\delta^{18}O$ ranges around –8‰). Waters with lower $\delta^{18}O$ values e.g. drilled wells have had a longer residence time in the ground and display values close to the annual average for precipitation of the area. The wells HLX01, HLX03 and HLX05 have a rather high HCO_3 content (above 300 mg/l) which indicate bacterial activity during closed/semi closed conditions which in turn implies a longer residence time in the ground. When plotting $\delta^{18}O$ versus $\delta^{2}H$ most of the analysed surface and shallow waters line up along the Meteoric water line (MWL) and display a variation in $\delta^{18}O$ between –11 and –8‰. The local annual average for precipitation is close to –10‰. The Baltic Sea sample collected outside (East) of the Upplångö island (see Figure 3-1) show $\delta^{18}O$ value of –6.4‰ whereas the samples collected along the Kärrsvik bay show values around –7.2‰. This indicates mixing of surface water which is also displayed by the lower Cl content in these samples (2,820 to 3,150 ppm Cl compared with 4,300 ppm Cl for the sample collected outside Upplångö). The added fresh water have $\delta^{18}O$ values which are somewhat higher than the annual mean average indicating a dominance of run-off.

The δ^{34}S-values show a variation between +17.8 and +19.2‰ for the four samples analysed from the HLX (01, 03, 04 and 08) boreholes at a depth of ~ 50 m, indicating a dominating marine source for that sulphur, possibly from marine sediments. Since most of the data are located within the calculated recharge areas on the mainland of Laxemar, a deep source for the sulphur is less probable. In order to explain the observed δ^{34}S values at least two processes accounting for the presence of the dissolved sulphate could be considered; a) sea-spray from the Baltic Sea reaching inland and b) leaching of sediments and/or till in the area by the recharge waters. Leaching of sediments is the more probable alternative. Three of the drilled wells sampled for δ^{34}S, show a very high bicarbonate contents (464 to 220 mg/l). These high bicarbonate values suggest microbial activity. Based on the sulphur isotope results, it can however, be concluded that sulphate reducing bacteria does not have a high activity in these samples. (In such case the δ^{34}S values are expected to be higher). During the installation of the soil tubes HS-gas was detected at some of sampling locations which generally is a good indication of ongoing microbial sulphate reduction. Unfortunately δ^{34}S was not sampled and analysed from these sampling points.

The shallow waters show generally a large variation in Si contents compared with variations in e.g. deep saline groundwater and Baltic Sea water. For example in some of the very diluted surface water up to 11 mg/l Si can be detected. However, in some of the other samples of very dilute water the Si contents are very low. This may be due to differences in contact time, in water/mineral ratios, and mineralogical compositions of the overburden. Along the flow paths the water becomes more and more rich in other ions and pH and Si contents stabilise. Groundwater is usually super-saturated in respect of quarts and slightly under-saturated in respect of amorphous silica and the deep groundwater has usually Si values around 6 mg/l.

Of special interest for this project is the finding that the trace elements Rb, Cs and Th seem to correlate with Cl (see Appendix 2 and Appendix 3). This may at first glance indicate a water conservative behaviour but since Cl can have several sources (deep saline and sea water) so can also trace elements be derived from several sources. The other trace elements seem to show an non-conservative behaviour which may be colloidal or different type of retardation due to water rock interactions.

5 M3 modelling

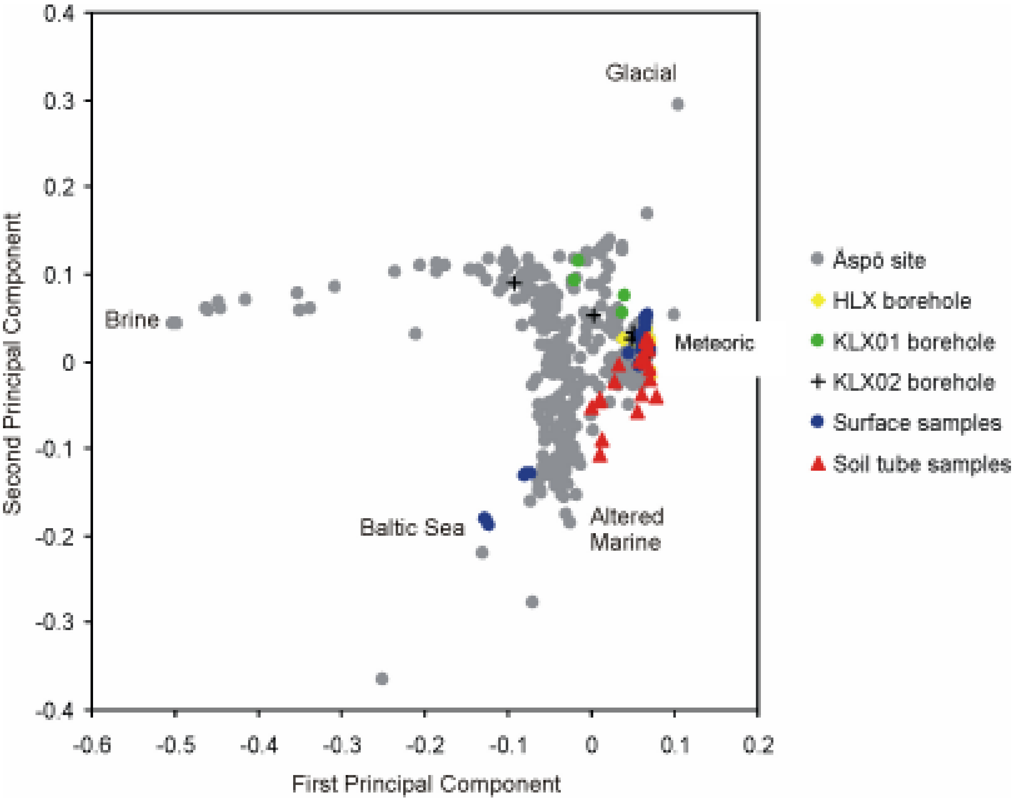
The M3 modelling (Multivariate Mixing and Mass-balance calculations) is a new modelling tool based on multivariate analysis /Laaksoharju et al. 1999a/. The first step in M3 modelling is a Principal Component Analysis (PCA) which aim at summarising the groundwater information from analytical data. The second step is a mixing calculation which aims at calculating the contribution from selected reference waters to the obtained groundwater composition. The third and final step is mass-balance calculations which indicate gains or losses due to reactions not accounted for by mixing. A mixing proportion of less than 10% is regarded as under the detection limit for the M3 method and is therefore uncertain. The M3 uncertainty range is ± 0.1 units at a confidence level of 90% based on an average uncertainty calculated over the polygon of interest. The modelling is always relative to the selected reference waters. M3 calculations can be used to indicate the following:

- Origin of the groundwater.
- Possible conceptual groundwater chemical model for the site.
- Major flow paths.
- Effects from reactions.
- Degree of dilution.
- Operational age of the groundwater.
- Element concentrations after compensating for contributions from various sources along the flow path.

In order to compare the selected 108 water samples with other samples from Äspö and Laxemar a PCA was performed (Figure 5-1). In M3 calculations for this data set ten variables were used: Na, K, Ca, Mg, HCO_3, Cl, SO_4^{2-}, $\delta^{18}O$, δ^2H and ^3H. The previously reported evaluation of the Äspö-Laxemar groundwater system /Laaksoharju and Wallin 1997, Laaksoharju et al. 1999b/ shows that at least five different water types can be recognised. These are: young meteoric water, Baltic Sea water (and older Litorina Sea water), Altered marine water (by sulphate reduction modified Sea water), Glacial meltwater/cold climate recharge and Brine type water (old saline water). The surface and shallow waters from the Laxemar area plot around the meteoric reference water. The Baltic Sea samples and the samples from the soil tubes plot between the meteoric and the Baltic Sea/Altered marine reference waters. The samples from KLX02 show the possible compositional flow path for deep groundwater and how the deep groundwater may intercept with shallow groundwater in the Biosphere.

A more local PCA has been made to model further the selected 108 water samples from Laxemar see Figure 5-2. The selected four reference waters: Deep Saline water, Meteoric, Surface water, and Baltic Sea water are:

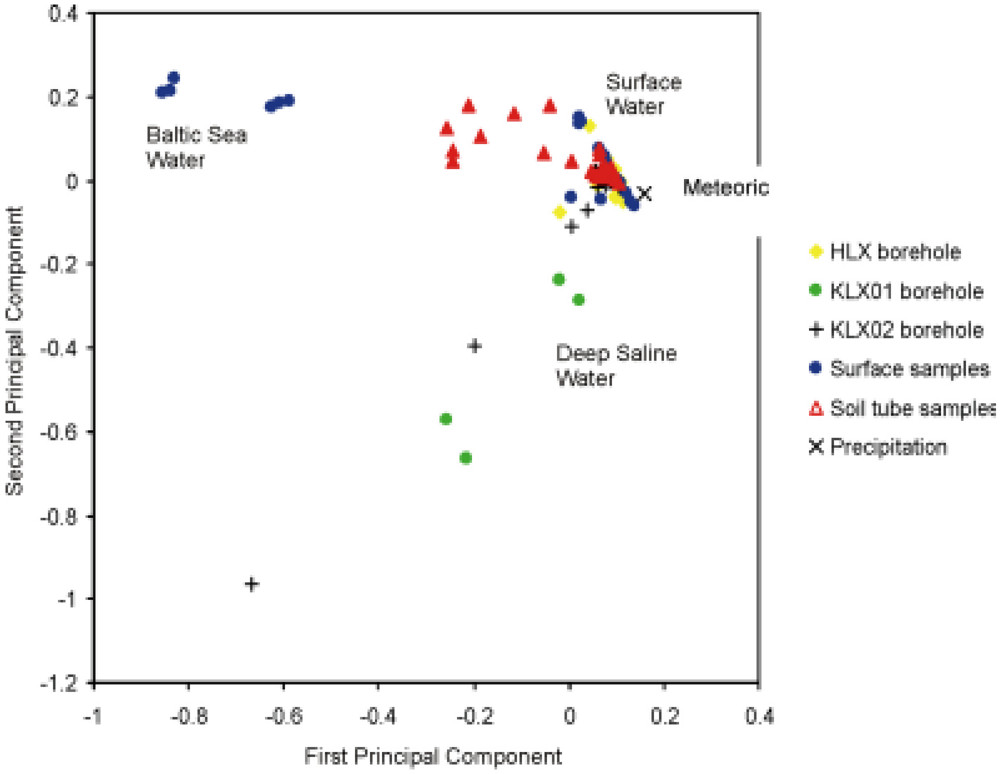
- Deep saline (no. 17 in Appendix 1) represents the KLX01 sample at 440 m depth.
- Baltic Sea water (no. 71 in Appendix 1) Sampled at the shore of Kråkemåla. Baltic Sea water is characterised by high values for major components especially for sodium, chloride and sulphate and by higher $\delta^{18}O$ and δ^2H values. The Baltic Sea waters sampled in the Kärrsviken bay plots close to the Baltic Sea reference water but have a significant portion of surface water.
- Surface water (no. 78 in Appendix 1) represents the PLX00037 sample representing the water from a ditch.
- Meteoric water (no. 108 in Appendix 1) represents the rain from 1960.



First principal Component = – 0.49[Na] + 0.04[K] – 0.01[Ca] – 0.007[Mg]+ 0.14[HCO_3] + 0.18[Cl] – 0.19[SO_4] + 0.02[O18] + 0.78[D] – 0.25[Tr]
Second Principal Component = – 0.28[Na] – 0.35[K] – 0.07[Ca] – 0.38[Mg]+ 0.10[HCO_3] – 0.79[Cl] + 0.14[SO_4] – 0.01[18O] + 0.04[D] + 0.002[Tr]

Figure 5-1. *Principal component plot for the selected 108 samples from Laxemar compared with data from the Äspö site. The samples plot along a meteoric-marine and meteoric-deep water (brine) mixing line. The variables Na, K, Ca, Mg, HCO3, Cl, SO4, $\delta^{18}O$ δ^2H and H_3 have been used in the PCA calculations. The reference waters Meteoric, Altered Marine, Baltic Sea, Glacial and Brine are indicated in the plot. The equations for the first respective second principal component are shown. In order to facilitate comparisons, the loadings for the different variables are normalised in M3 since this is how eigenvectors are generally presented. The elements are centre scaled before eigenvalues and eigenvectors are calculated. This means that e.g. [Na] is not the concentration of Na, but the standardised concentration of Na. The first and second principal components summarise 70% of the total information in the variables.*

The closer a sample in the PCA is to a reference water the more similar is the water composition. This is used in the mixing calculations where the distance to the reference water is equivalent to the mixing portion. The samples outside the polygon are not used for further M3 modelling. The calculated mixing proportions are listed in Appendix 1. For testing purposes additional variables were inserted in the PCA, such as the elevation and the distance from the sampling points to the sea (see Appendix 5). The new PCA shows a slight difference compared with the PCA in Figure 5-2 (the soil tube samples seems to group and may form a 5th end member), but the overall interpretation can be considered similar. Elements such as nitrate and phosphate could have been useful tracers for surface water input unfortunately the data set contains only a few measurements (6 values for NO_3-N and 15 values for PO_4-P, see Appendix1), which invalidates the use of PCA.



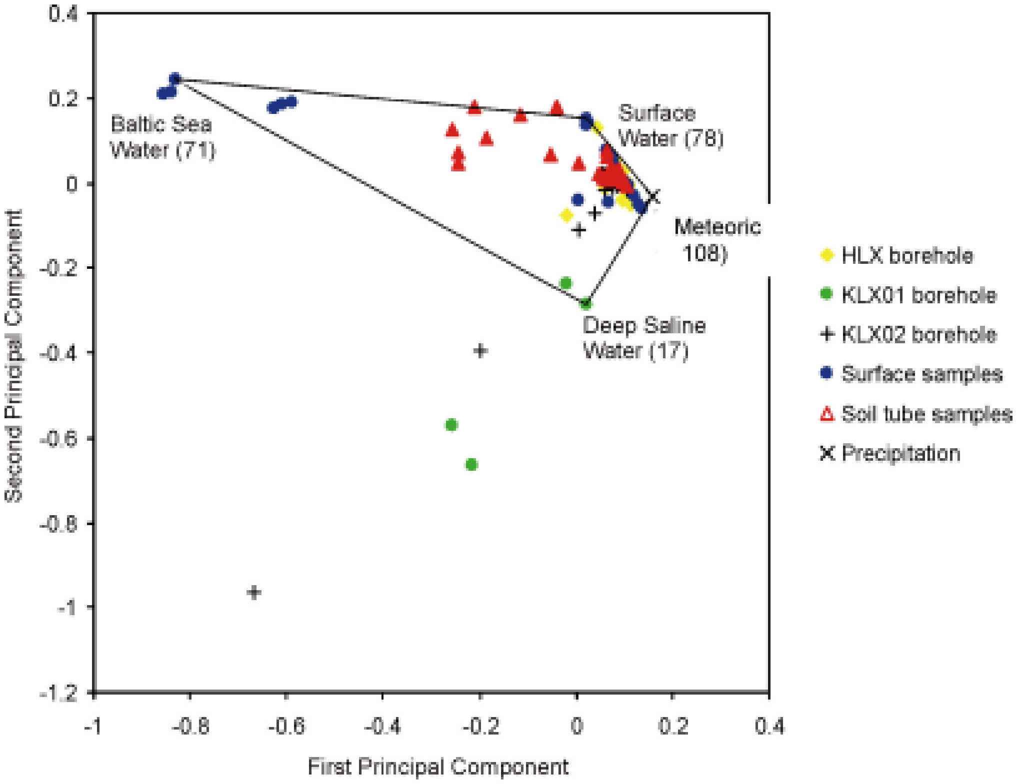
First Principal Component = – 0.42[Na] – 0.22[K] – 0.04[Ca] – 0.05[Mg]–
0.17[HCO_3] + 0.14[Cl] – 0.11[SO_4] – 0.06[O18] – 0.70[D] + 0.46[Tr]
Second Principal Component = – 0.42[Na] + 0.18[K] – 0.11[Ca] – 0.15[Mg]–
0.30[HCO_3] + 0.10[Cl] – 0.39[SO_4] – 0.60[O18] + 0.37[D] – 0.06[Tr]

Figure 5-2. *Principal component plot based on the 108-sampled surface/shallow water data together with Laxemar data to a depth of 1,000 m. The samples plot along a meteoric-marine and meteoric-deep saline water mixing line. The variables analysed are Na, K, Ca, Mg, HCO3, Cl, SO4, $\delta^{18}O$, $\delta^{2}H$ and ^{3}H. The first and second principal components summarise 73% of the total information in the variables. The reference waters Meteoric, Surface, Baltic Sea, and Deep Saline are indicated in the plot.*

A detailed examination of the PCA (Figure 5-3) shows that some shallow samples with higher Cl content e.g. observations 64 and 84 (for orientation see the PCA in Appendix 1) of these only sample 84 was affected by some deep saline groundwater (24%) the other sample no: 64 (3%) was under the detection limit for the M3 method which is 10%. This may anyhow indicate an influence of deeper saline waters (the reference water used in this modelling was KLX01 at –440 m depth) into the shallow groundwater that cannot be ruled out. There are a total of observations from the surface and shallow samples which have a calculated mixing portion of Deep Saline groundwater that is more than 10%. These observations are all along the major fracture zone of the modelled area (see Figure 5-4, the red circles) where the hydro modelling indicated discharge of deep groundwater.

If there is a transport from the deep groundwater up to the biosphere the dilution is expected to be large. A calculation was made based on the M3 mixing calculations. Where the following assumptions where made:

1) Based on the results from M3 mixing calculations a dilution calculation was made from the “repository depth” which is represented by KLX01:440 m (The Deep Saline reference water).
2) The Cl is transported in a water conservative way from the “repository” up to the biosphere.



First Principal Component = – 0.42[Na] – 0.22[K] – 0.04[Ca] – 0.05[Mg]– 0.17[HCO_3] + 0.14[Cl] – 0.11[SO_4] – 0.06[O18] – 0.70[D] + 0.46[Tr]
Second Principal Component = – 0.42[Na] + 0.18[K] – 0.11[Ca] – 0.15[Mg]– 0.30[HCO_3] + 0.10[Cl] – 0.39[SO_4] – 0.60[O18] + 0.37[D] – 0.06[Tr]

Figure 5-3. *Principal component plot based on the 108 sampled surface/shallow water data together with Laxemar data to a depth of 1,000 m. The variables analysed are Na, K, Ca, Mg, HCO3, Cl, SO4, $\delta^{18}O$, $\delta^{2}H$ and ^{3}H. The first and second principal components summarise 73% of the total information in the variables. The reference waters Meteoric, Surface, Baltic Sea, and Deep Saline are indicated in the plot. The polygon shows the modelled area which is used with M3 to determine the mixing proportions from the reference waters to the obtained water compositions. Only observations inside the polygon can be used for further M3 modelling.*

Based on the above assumptions the contribution of Cl from the repository depth up to the surface and shallow samples where calculated and compensated for influences from other saline sources such as Baltic sea water. The calculated results are shown in Appendix 1 and the mean Cl contribution from the repository depth to the shallow and surface groundwater is 1.38% (maximum = 14.32%, minimum = 0.003%). This means that if a water conservative tracer would be transported up to the surface during prevailing hydrogeological conditions generally less than 2% of the original concentration will reach the groundwater in contact with the biosphere. The average dilution is generally more than 98%.

Another important issue is the operational age of the mixing proportions, which reflects how fast a tracer can be transported from depth up to the biosphere. For this calculation the M3 mixing proportions where used and the following assumptions where made:

1) Since we assume that the water consists of a mixture of different reference waters, by giving the reference waters an age the age contribution to the mixture water can be calculated.
2) Several tests were made with the following ages given to the reference waters:
   Meteoric = 40 years alternatively 0 years, Surface = 0 years, Baltic Sea = 3,000 or 0 years and Deep Saline = 10,000 years or 100,000 years.

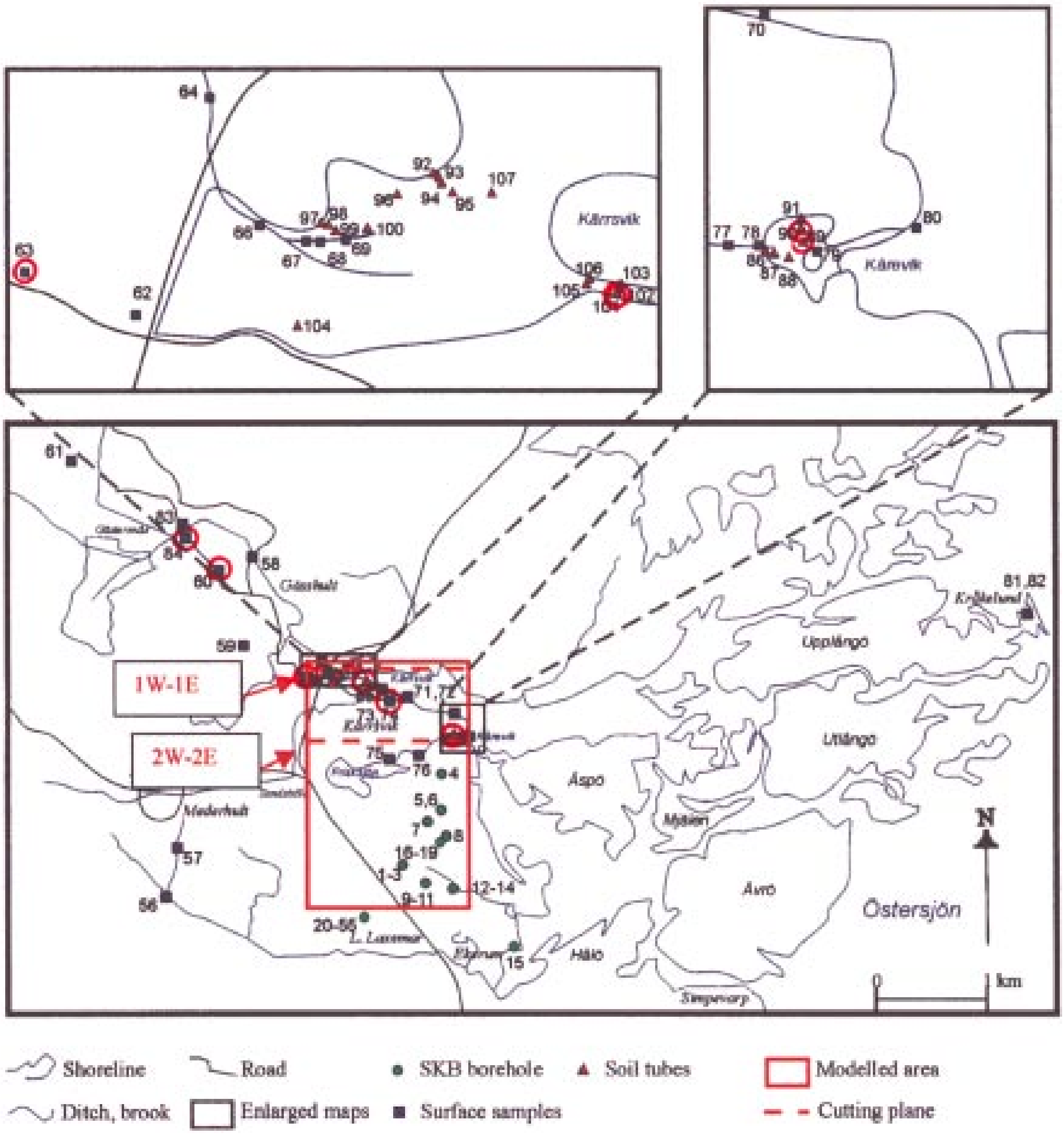


Figure 5-4. *Map showing the surface and shallow samples (red circle) with a calculated contribution of Deep saline groundwater witch exceeds 10%. These samples can have an influence from the deep groundwater.*

The calculated operational age was from 100,000 years (at 1,000 m depth) to 10,000 years (at 500 m depth) up to 8 years for surface water (at 1 m depth). The results of the following calculations are presented in Appendix 1: deep saline = 10,000 years, Baltic = 3,000 or 0 years, Surface = 0 years, Meteoric = 60 years. The results from the above calculations should be seen as a rough estimate.

6 Visualisation of the measured and modelled domain

As shown in the Figure 3-1, several modelled domains were set up. The reason to build different models is to better understand the interaction of the hydro-geo-chemical system at different depth and time scales (by using different reference waters) but also to test the robustness of the modelling approaches.

The models presented and studied in this work are:

- **Superficial box:** represented by the red square in the Figure 3-1, with the depth of 56 m (see Section 6.1 below).
- **Deep box:** represented by the red square in the Figure 3-1, with the depth of 500 m (see Section 6.2 below).
- **Enlarged box:** represented by the black square in the Figure 3-1, with the depth of 500 m (see Appendix 6).
- **Very deep box:** the enlarged box and the deep box are extended to 1,000 m (see Appendix 6).

6.1 Superficial box

In order to show graphically the results of the measured and M3 calculated values a visualisation was performed for two 56 m deep vertical cross-sections trough the modelled area. The cross-sections are named profile 1 (1W-1E) and 2 (2W-2E) (for orientation see Figure 3-1). The 3D interpolation in this work was always performed by using the computer code Voxel Analyst by INTERGRAPH. The following features of the profile 1 and 2 and the transects NW-SE were visualized as follows:

- Measured values of: Cl, EC (electrical conductivity), Na, Ca and oxygen-18.
- Calculated mixing proportions with M3 of Meteoric, Shallow, Baltic and Deep saline waters.
- Operational age calculated based on the mixing of the different water types with given ages.
- Measured and the M3 calculated deviation of the elements HCO_3 and SO_4 (positive value = gain, negative value = loss of element accounted for by reactions).

The M3 modelling is based solely on chemical information that can be used to support the understanding of groundwater flow through the site area. The calculated mixing proportions are always relative to the selected reference water. The results of the Voxel interpolations are shown in Figures (6-1 to 6-12). The topography along the profiles is shown in all the figures. The numerical values of the M3 mixing and deviation calculations for all observations are listed in Appendix 1.

The M3 modelling indicates that the surface and shallow groundwater system is complex. The upper groundwater system includes interaction between different water types and reactions such as inorganic and biogenic reactions. These mechanisms may also make the tracking of trace elements difficult since the original content is altered.

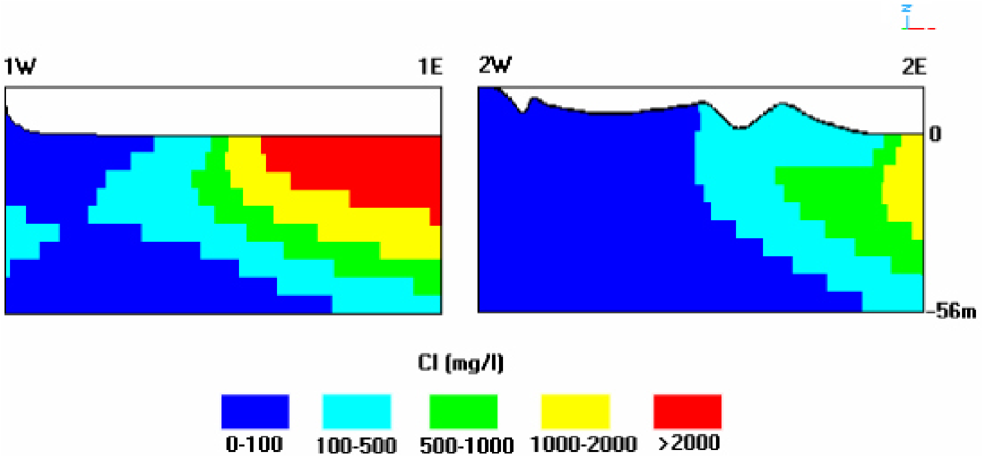


__Figure 6-1.__ Result of the Cl interpolation of measured values along the profile 1 (1W-1E) and 2 (2W-2E) (for orientation see Figure 3-1). Profile 1 indicates a possible interaction of salinity contribution from deeper water (lower left part of the profile). The upper right part of the profiles represents influences of Baltic Sea water.

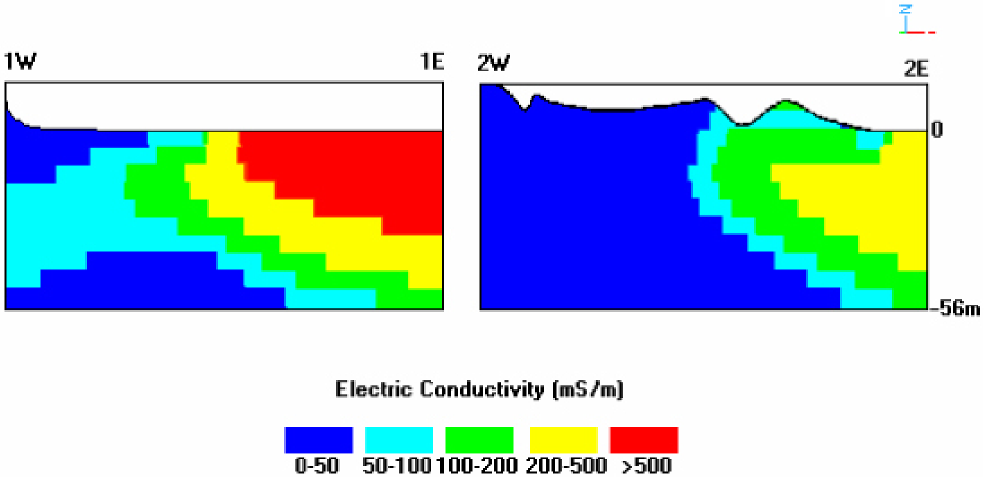


__Figure 6-2.__ Result of the electrical conductivity interpolation of measured values along the profile 1 and 2 (for orientation see Figure 3-1). Profile 1 indicates a possible interaction of more saline (more conductive) from deeper water (lower left part of the profile). The upper right part of the profiles represents influences of Baltic Sea water.

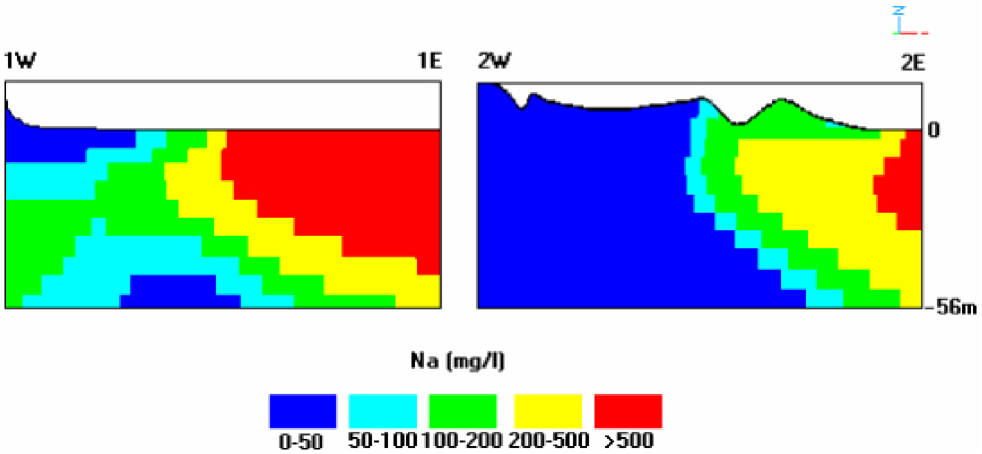


__Figure 6-3.__ Result of the Na interpolation of measured values along the profile 1 and 2 (for orientation see Figure 3-1). Profile 1 indicates a possible interaction of more saline (more conductive) from deeper water (lower left part of the profile). The upper right part of the profiles represents influences of Baltic Sea water.

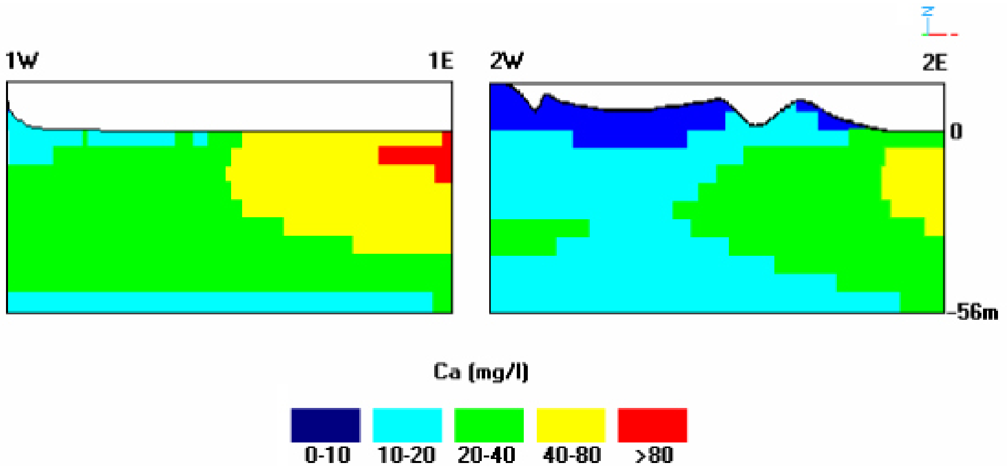


Figure 6-4. *Result of the Ca interpolation of measured values along the profile 1 and 2 (for orientation see Figure 3-1). Profile 1 and 2 indicate a complex source for Ca possible from Sea Water (upper right part of the profiles) and also from possible reactions such as calcite dissolution.*

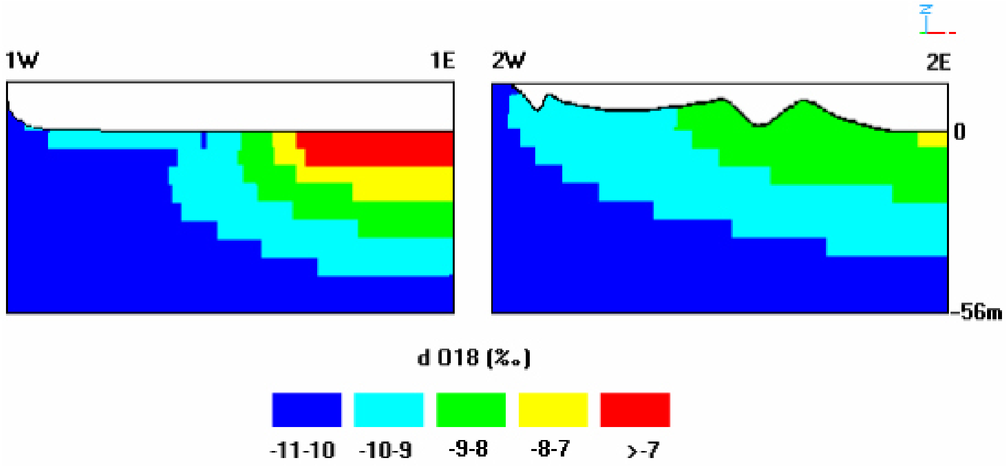


Figure 6-5. *Result of the oxygen-18 interpolation of measured values along the profile 1 and 2 (for orientation see Figure 3-1). Profile 1 and 2 indicate a higher value for water associated with Baltic Sea water and a lower value for surface and shallow water. The lower the value the longer the operational age of the water is believed to be. The mean value of the annual precipitation is –10.*

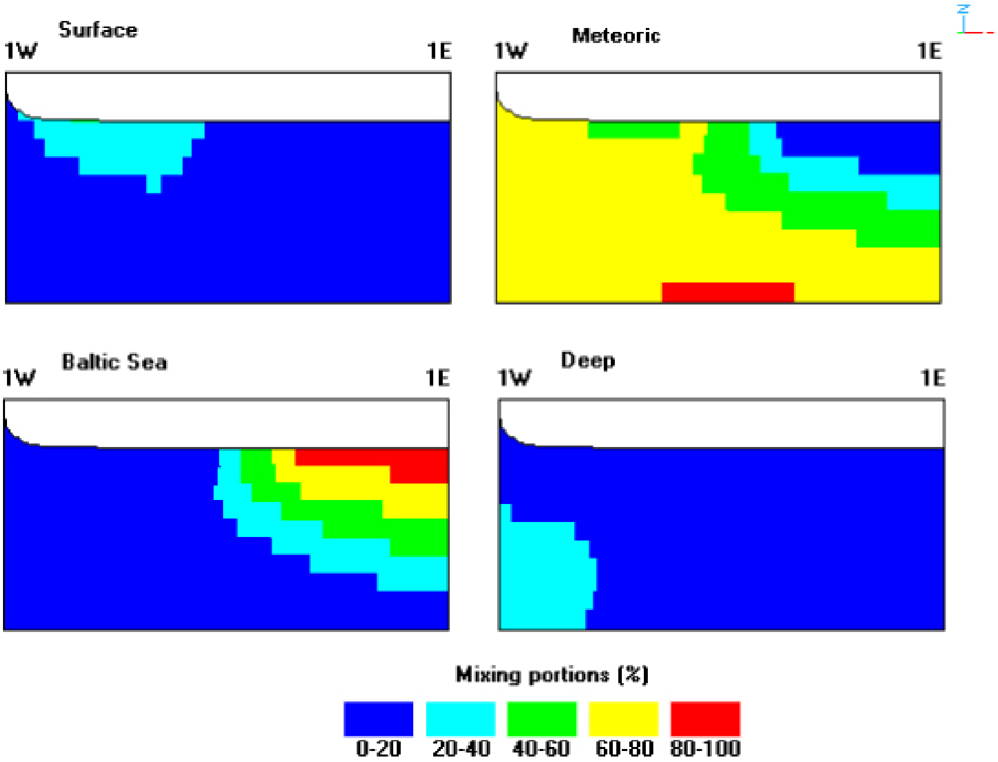


Figure 6-6. Result of interpolation of calculated mixing proportions based on M3 calculations for Surface, Meteoric, Baltic Sea, and Deep Saline water along the profile 1 (for orientation see Figure 3-1). There is an indication of deep water influences in the lower right part of the profile.

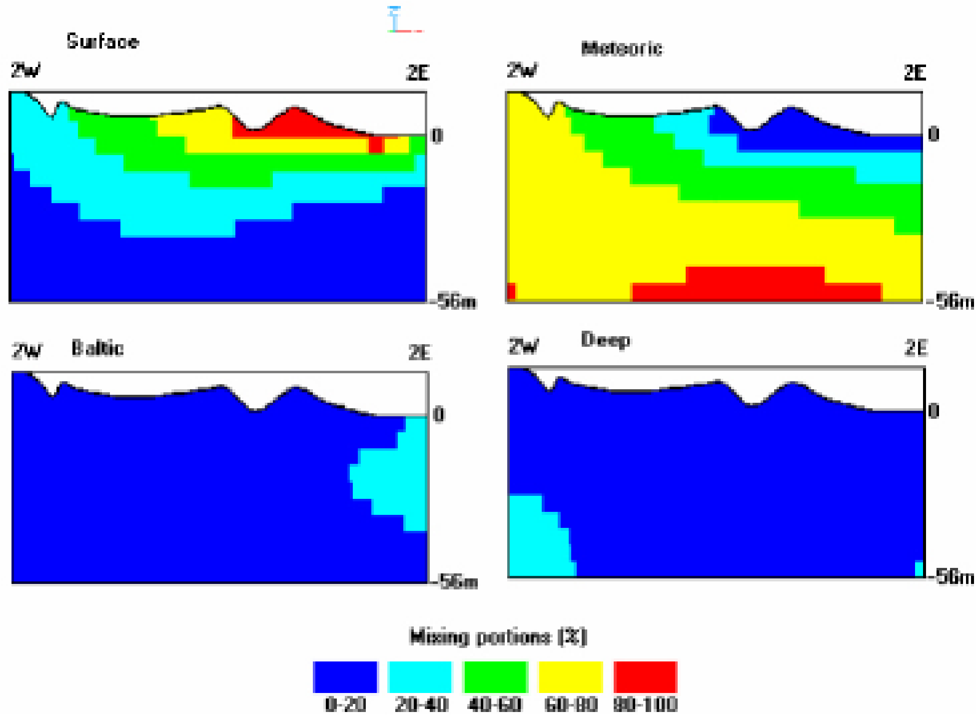


Figure 6-7. Result of interpolation of calculated mixing proportions based on M3 calculations for Surface, Meteoric, Baltic Sea, and Deep Saline water along the profile no: 1 (profile 1W-1E, for orientation see Figure 3-1). There is an indication of deep water influences in the lower right part of the profile.

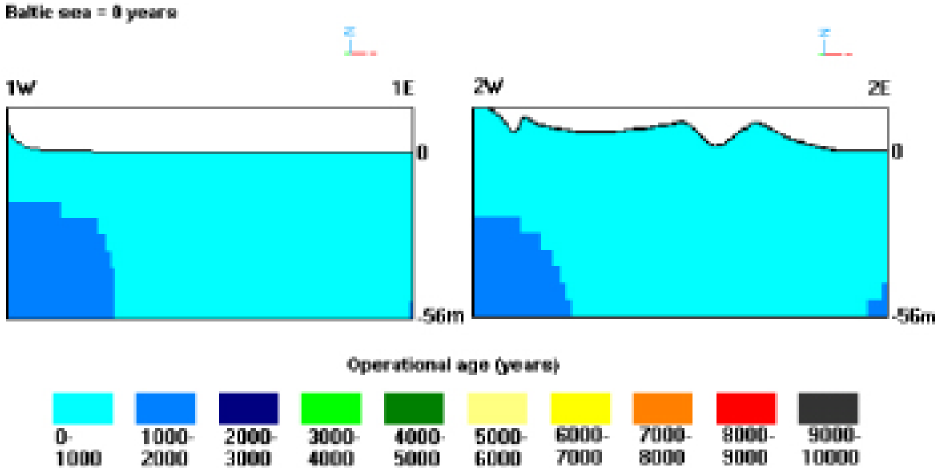


***Figure 6-8.** Result of the Operational age interpolation of calculated values along the profile 1 and 2 (for orientation see Figure 3-1). In this example, the Surface water and the Baltic Sea water = 0 years, the meteoric water = 40 years and the deep saline water = 10,000 years. The modelling indicates that the operational age at 56 m depth can vary between 0 to 2,000 years when using these assumptions.*

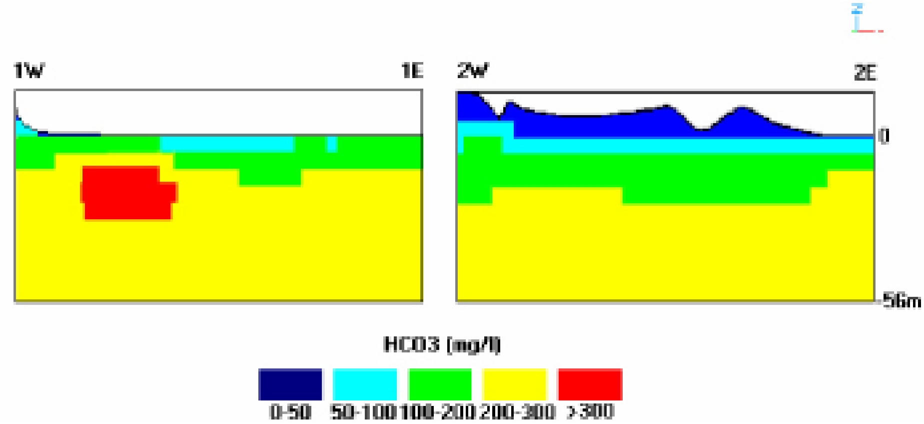


***Figure 6-9.** Result of the HCO_3 interpolation of measured values along the profile 1 and 2 (for orientation see Figure 3-1). Profile 1 and 2 indicate a complex source for the measured HCO_3 content.*

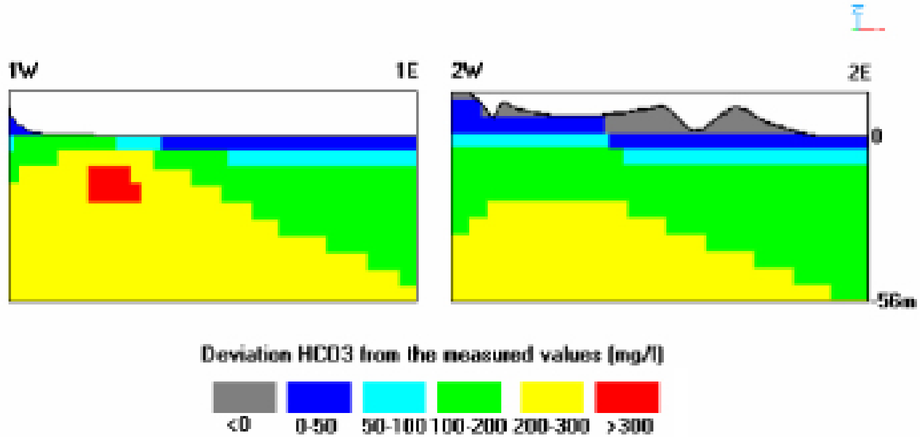


***Figure 6-10.** Result of the HCO_3 interpolation of calculated M3 deviation values not accounted for by transport. A positive value indicates gain a negative value a loss possible due to reactions. Profile 1 and 2 indicate a complex gain of HCO_3 possible from biogenic activity or calcite dissolution. Sulphate reduction associated with the Marine sediments can cause a gain of dissolved HCO_3 in the groundwater. The potential seems to be higher for profile 1 compared with profile 2.*

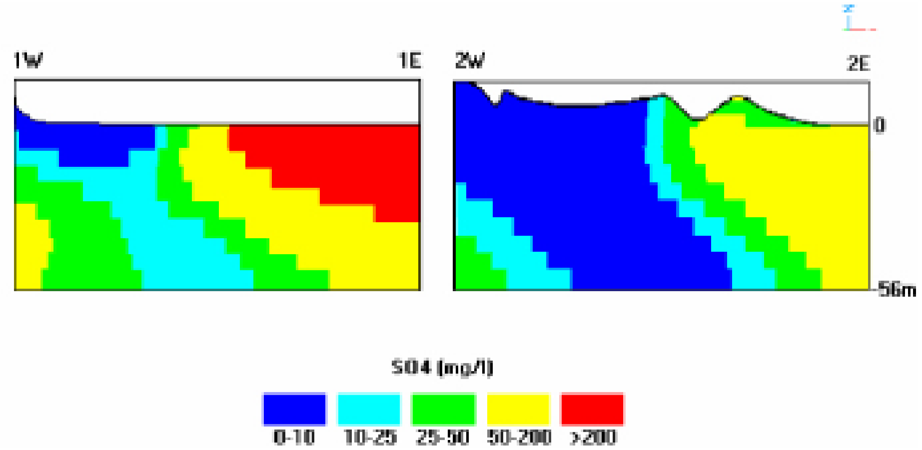


Figure 6-11. *Result of the* SO_4 *interpolation of measured values along the profile 1 and 2 (for orientation see Figure 3-1). Profile 1 and 2 indicate a complex source for the measured* SO_4 *both from Sea and Deep water.*

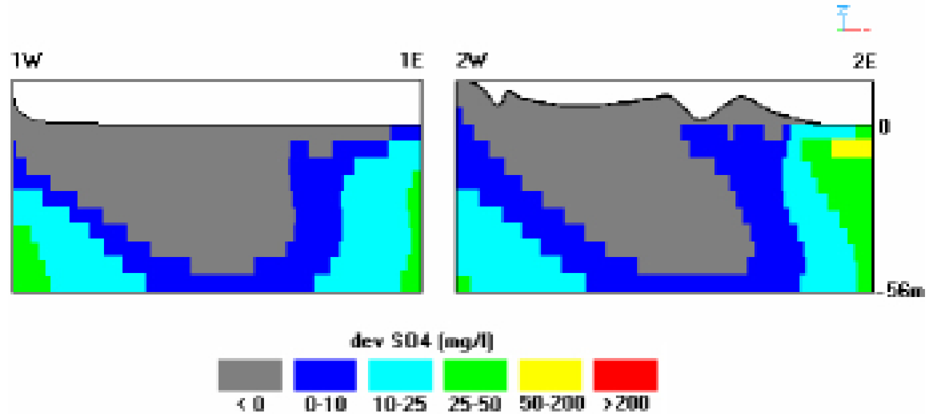


Figure 6-12. *Result of the* SO_4 *interpolation of calculated M3 deviation values not accounted for by transport. A positive value indicates a gain a negative value a loss possible due to reactions. Profile 1 and 2 indicate a gain of* SO_4 *below the Sea and from the Deep water. A loss is indicated in the middle and upper part of the profiles. Areas with loss of* SO_4 *in combination with gain of* HCO_3 *(cf. Figure 6-9) can indicate areas with sulphate reduction associated with the marine sediments.*

6.2 Deep box

For comparison the modelled area presented in the pervious Section (6.1) was extended to a depth of 500 m and named the "Deep box". The cross-sections are named profile 1 (1W-1E) and 2 (2W-2E). The modelling was completed by adding two cross-sections NW-SE and 3W-3E (for orientation see Figures 6-13 and 3-1). The following features of the profiles were visualised:

- Measured values of: Cl and oxygen-18.
- Calculated mixing proportions with M3 of Meteoric, Shallow, Baltic and Deep saline waters (the same deep saline water as used in the model "superficial box" was used as a reference water).
- Calculated values of the operational age based on the reference water ages.
- Measured and M3 calculated deviation of the elements HCO_3, SO_4 and Ca (positive value = gain, negative value = loss of element content accounted by reactions).

The calculated mixing proportions are always relative to the selected reference waters. The results of the Voxel interpolations are shown in Figures (6-13 to 6-21). The results of the M3 mixing and deviation calculations for all observations are listed in Appendix 1.

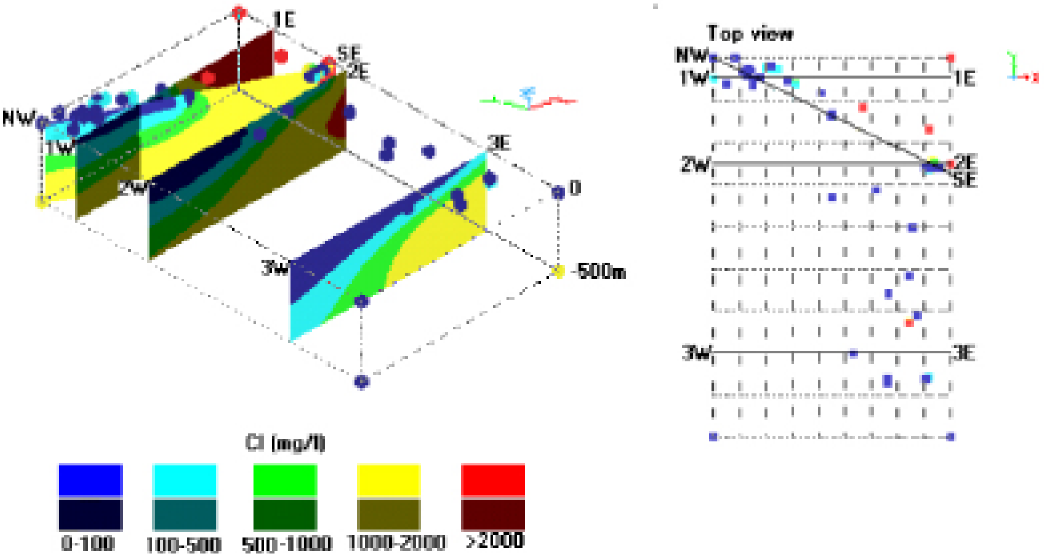


***Figure 6-13.** Visualisation of the sampling points, interpolation grid and location of the cutting planes 1(1W-1E), 2 (2W-2E), 3 (3W-3E) and the transect NW-SE (for orientation see Figure 3-1). A perspective view (left figure) and a top view (right figure) are presented. The concentration of Cl is shown in the sampling points, as well as along the cutting planes. Note that the 2 colour scales were used for visualisation purposes to show front light and shadow.*

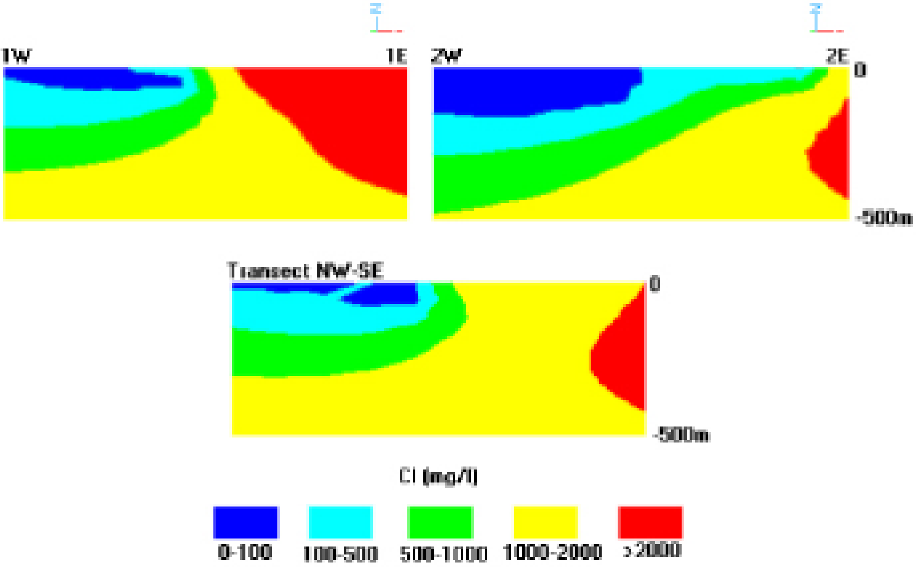


***Figure 6-14.** Result of the Cl interpolation of measured values along the profiles 1 and 2 and transect NW-SE (for orientation see Figures 6-13 and 3-1). Profile 2 indicates a possible interaction of salinity contribution from deeper water (lower left part of the profile). The upper right part of the profiles represents influences of Baltic Sea water. To be noticed is the difference between Cl distribution, operational age (Figure 6-18) and the deep saline water distribution (Figure 6-17). This can indicate that the Cl can have different origins and ages.*

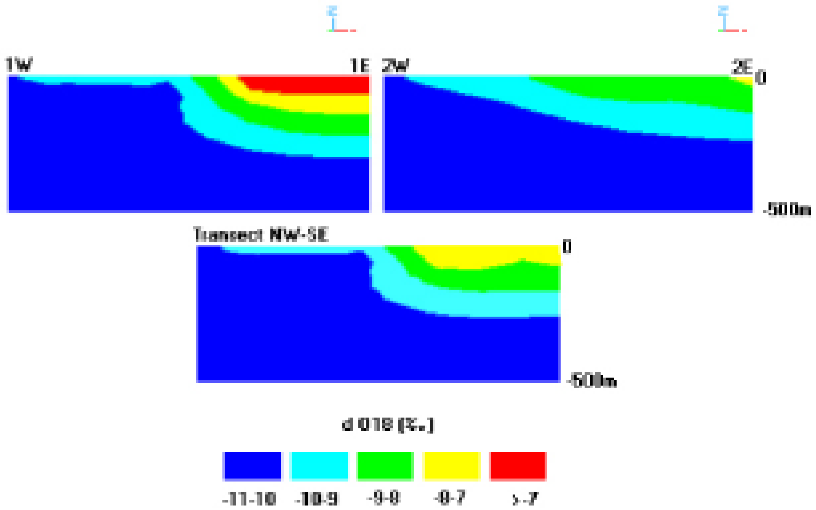


Figure 6-15. *Result of the oxygen-18 interpolation of measured values along the profile 1, 2 and transect NW-SE (for orientation see Figures 6-13 and 3-1). The profiles indicate a higher value for water associated with Baltic Sea water and a lower value for surface and shallow water. The mean value of* $\delta^{18}O$ *of the annual precipitation is –10.*

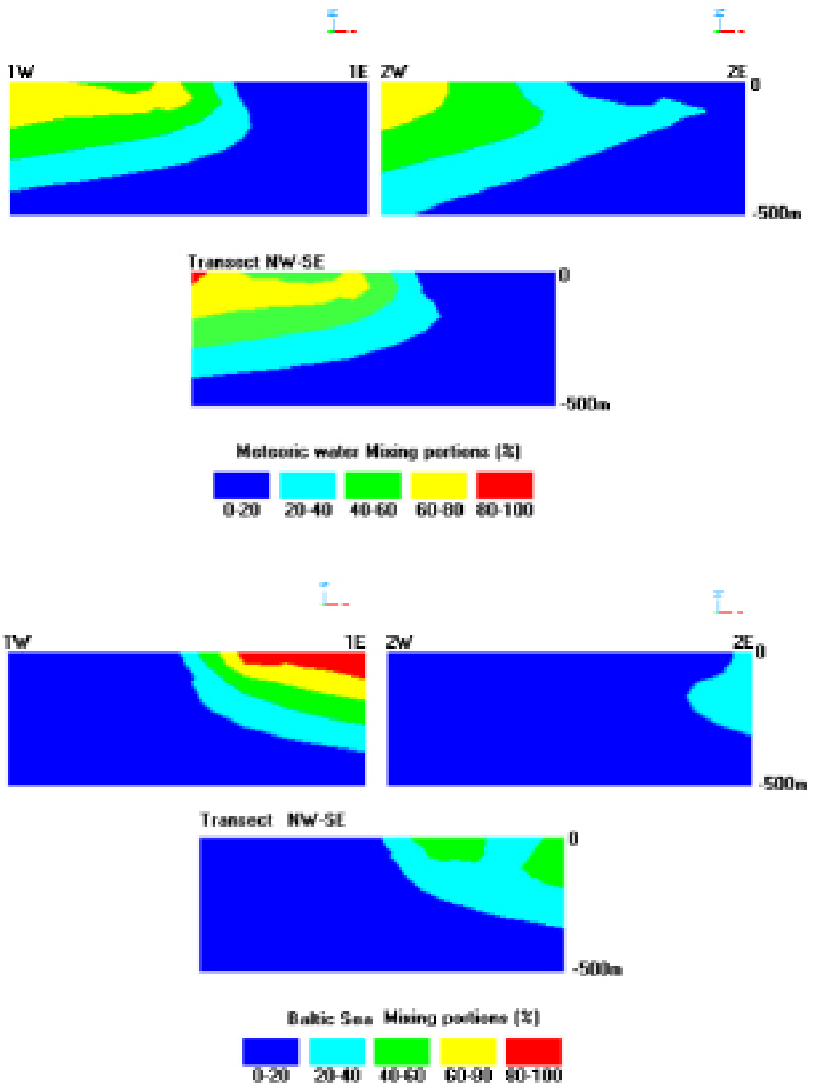


Figure 6-16. *Result of interpolation of calculated mixing proportions based on M3 calculations for Meteoric and Baltic Sea water along the profiles 1W-1E, 2W-2E and the transect NW-SE (for orientation see Figure 6-13 and 3-1).*

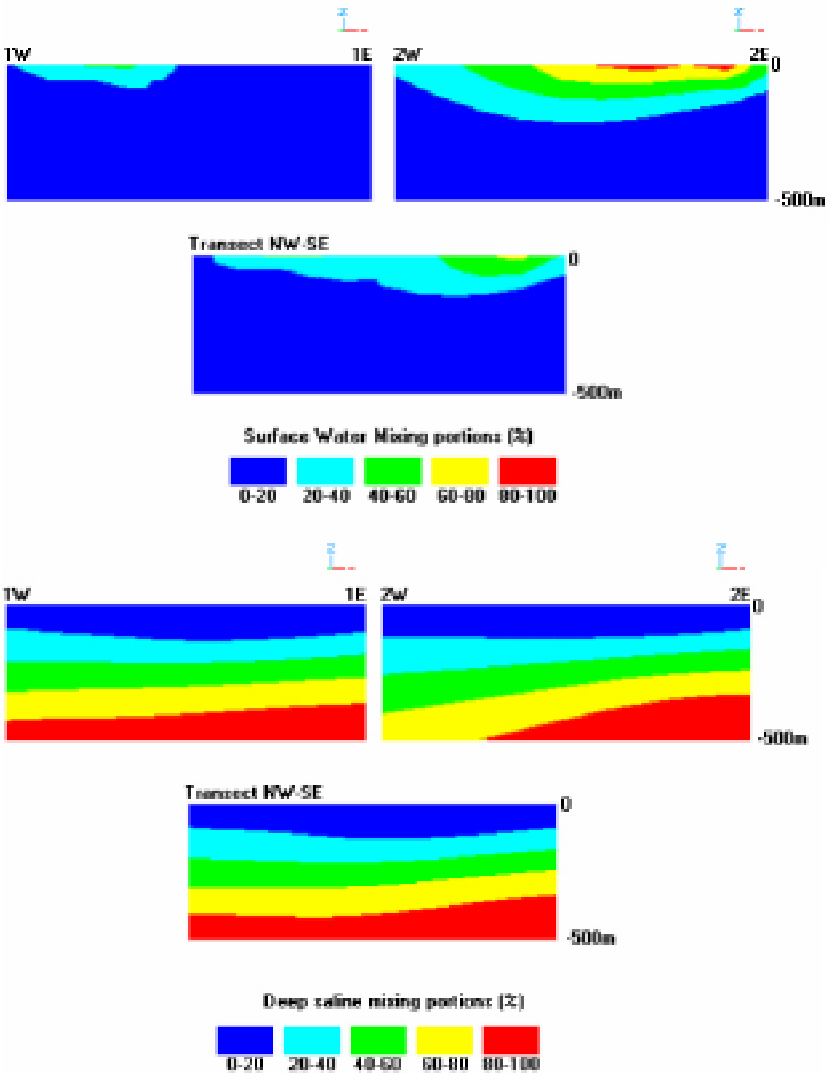


Figure 6-17. *Result of interpolation of calculated mixing proportions based on M3 calculations for Surface and Deep Saline water along the profiles 1W-1E, 2W-2E and the transect NW-SE (for orientation see Figures 6-13 and 3-1).*

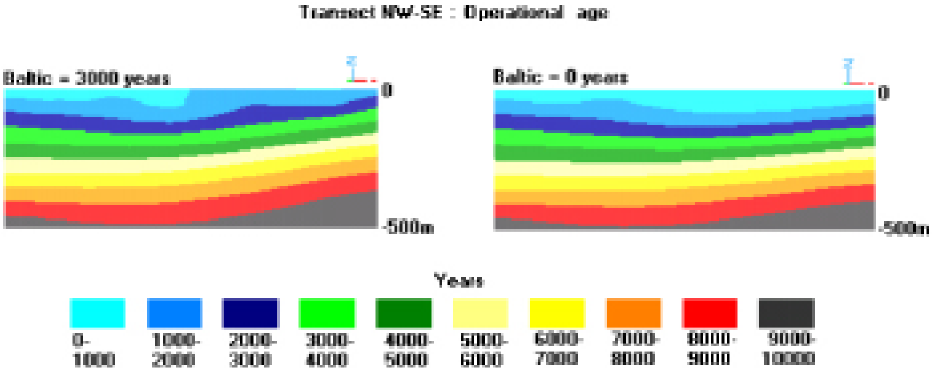


Figure 6-18. *Result of the calculated operational age along the transect NW-SE (for orientation see Figure 6-13 and 3-1) based on the reference waters ages: Meteoric water = 40 years, Surface water = 0 years, Deep saline water = 10,000 years. For the Baltic Sea water two cases were considered: Baltic Sea = 3,000 years (the left model assumes that the Baltic sea has been residing in the bedrock since the land elevation) and Baltic Sea = 0 years (right model assumes that the sea water in the bedrock is modern). When using the assumed age 3,000 years for the Baltic Sea (left model), it is observed that the bedrock can contain older water at a lower depth compared with a model using a modern Baltic sea water of 0 year (right model). Both models show an increase of the operational age with depth. The operational age has the same distribution as the calculated mixing distribution of deep saline water (cf. Figure 6-17).*

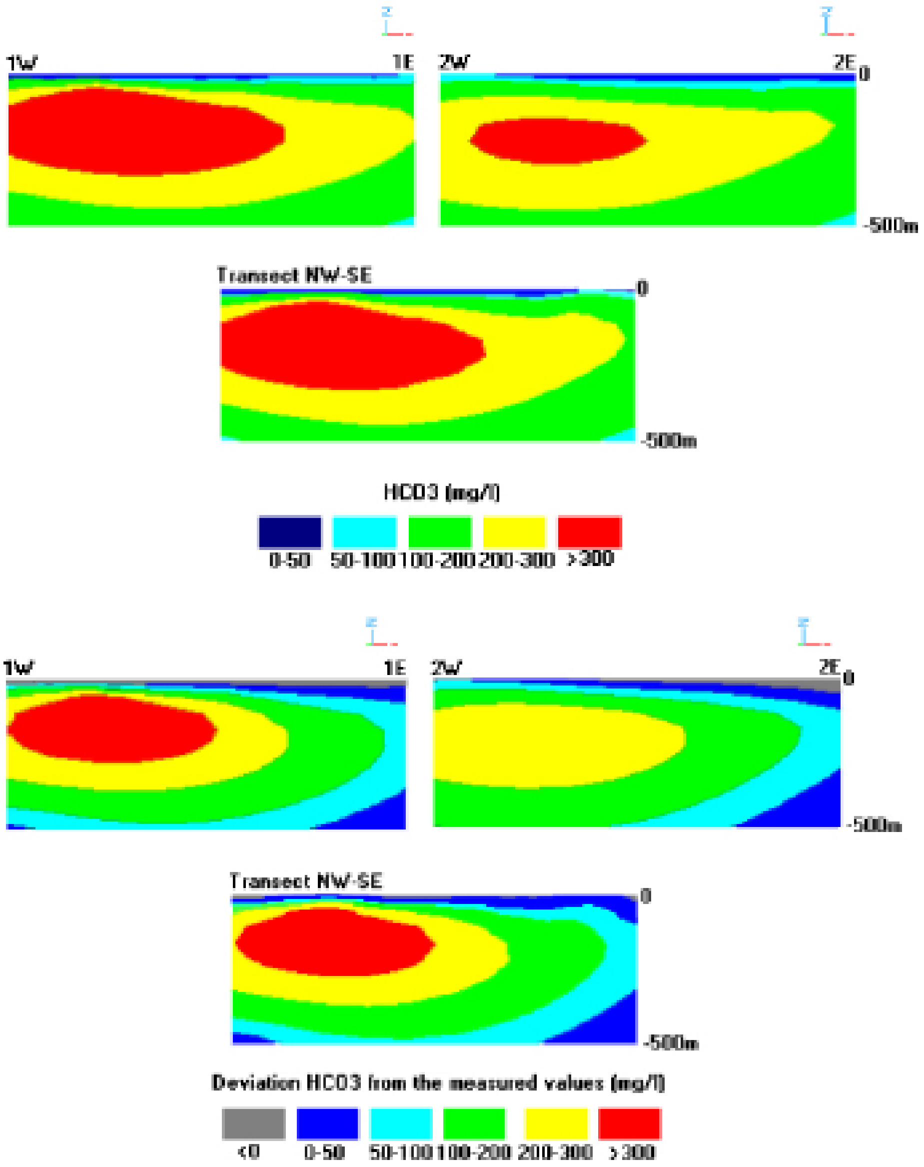


Figure 6-19. *Result of the HCO_3 interpolation of measured values along the profile 1 and 2 and the transect NW-SE (for orientation see Figures 6-13 and 3-1). Profile 1, 2 and the transect NW-SE indicate a complex source for the measured HCO_3 content. The lower figures show the HCO_3 deviation not accounted for by mixing in M3. A positive value indicates gain and a negative value a loss possible due to reactions. Profile 1, 2 and transect NW-SE indicate a gain of HCO_3 possible from biogenic activity or calcite dissolution. Sulphate reduction associated with the Marine sediments can also cause a gain of dissolved HCO_3 in the groundwater. The potential seems to be higher for profile 1 and transect NW-SE compared with profile 2.*

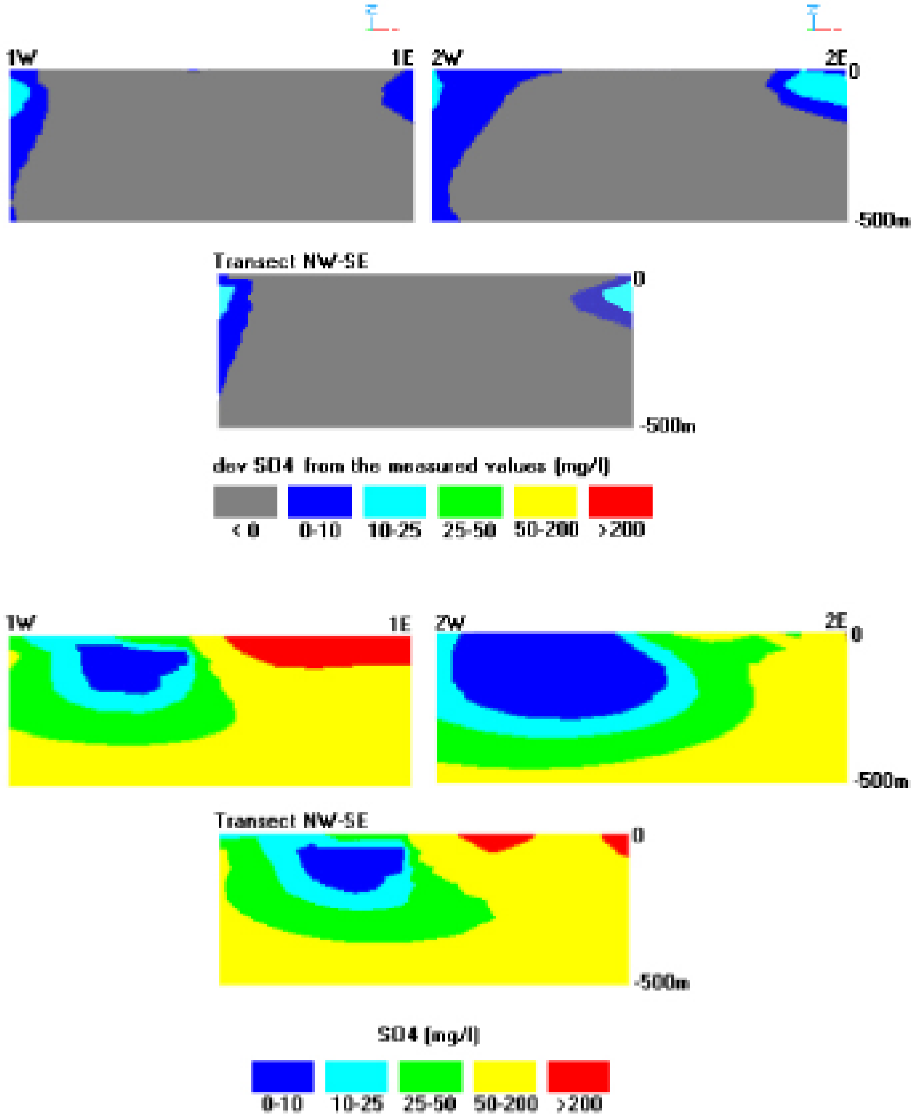


Figure 6-20. *Result of the SO_4 interpolation of measured values (upper figures) along the profile 1, 2 and transect NW-SE (for orientation see Figures 6-13 and 3-1). The profiles indicate a complex source for the measured SO_4 both from Sea and Deep water. The lower figures show SO_4 deviation not accounted for by transport in M3. A positive value indicate a gain a negative value a loss possible due to reactions. The profiles indicate a gain of SO_4 below the Sea and from the Deep water. A loss is indicated in the middle and upper part of the profiles. Areas with loss of SO_4 in combination with gain of HCO_3 (cf. Figure 6-19) can indicate areas with sulphate reduction associated with the marine sediments.*

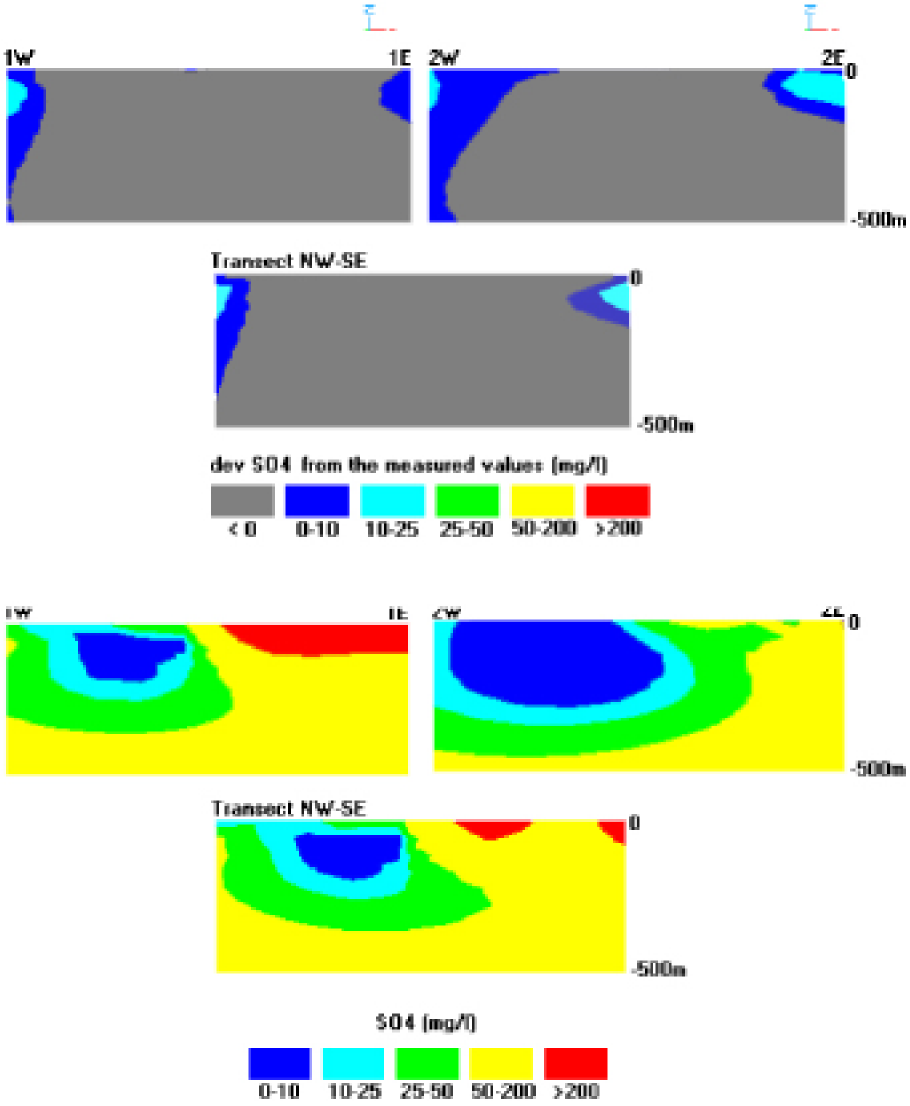


Figure 6-21. Result of the Ca interpolation of measured values (upper figures) along the profiles 1, 2 and transect NW-SE (for orientation see Figures 6-13 and 3-1). The profiles 1, 2 and NW-SE indicate a complex source for Ca possible from Sea Water (upper right part of the profiles) and also from possible reactions such as calcite dissolution. Lower figures show the deviation for Ca not accounted for by transport in M3 calculations. A positive value indicates a gain a negative value a loss possible due to reactions. The profiles indicate a loss of Ca at the surface. A gain is indicated in the middle and lower part of the profiles.

The M3 modelling indicates that the interaction between surface-, shallow- and deep groundwater system is complex. The upper groundwater system includes interaction between different water types and reactions such as inorganic and biogenic reactions. Many of the reactions taking place in the surface and shallow groundwaters may act as a retardation mechanism for the transport of many radionuclides. The Cl, used in classical modelling as a good conservative tracer, cannot alone be used as a tracer in this complex system since Cl can have many sources such as modern/ancient seawater and brine type of water. This is put in evidence by the fact that the operational age is not correlated with the Cl. The operational age is only correlated with the deep saline water type. The visualisation of the extended profile towards NW (Enlarged box) and the extended box towards the depth of 1,000 m (Very deep box) are presented in Appendix 6. The general conclusion from extending the modelled area is that despite changing the scale the overall interpretations of the modelling remains unchanged.

7 Conclusions

A total of 108 surface, shallow and deep groundwater samples were studied from the Laxemar area close to Äspö Hard Rock Laboratory. According to the hydrological modelling /Svensson 1997/ the transport process of deep groundwater may be induced by a possible regional flow, pumping actions from changes in groundwater and sea levels. A conclusive indication of interaction between deep groundwater and shallow groundwater cannot be made from studying chemical data. The sampling, analytical and modelling difficulties together with the unknown effect on the regional flow from the Äspö HRL tunnel construction (Ingvar Rhen, pers. comm. 2006) make any comprehensive conclusions difficult which is the main conclusion of this work.

In order to visualise different aspects of the M3 modelling results, several models were set up. The reason to build different models is to better understand the dynamics of the hydrogeochemical system at different scales in space (at surface and depth) and time (different reference waters). The conclusions from these tests are that despite changing the scale from 50 to 1,000 m the results are similar. All the modelling indicates a possibility for interaction but also a large dilution and long transport times from the repository depth to the surface. Chloride, which generally thought to be a water conservative tracer is not a reliable tracer in this case since the Cl can have several sources.

The M3 modelling indicates that there are 8 shallow samples which had a larger than 10% calculated contribution from deep groundwater (500 m). These observations are all from the major fracture and discharge area in the modelled area. The conclusion is therefore that deeper groundwater could be in contact with shallow and surface water in discharge areas close to the coast as described by the hydrogeological modelling. The major conclusions from the study are:

- The upper groundwater system includes interaction between different water types and contributions from inorganic and biogenic reactions. Many of the reactions taking place in the surface and shallow groundwaters may act as a retardation mechanism for the transport of many elements. The influences from deep groundwater cannot be ruled out but the mixing, dilution and reactions taking place in the upper hydrodynamic active parts makes the transport effects difficult to trace.
- An operational age of groundwater is defined from the mixing proportions and reflects a possible average residence time for the water. Calculation of the operational age for the groundwater at the repository depth to the surface indicated that the waters could have an operational age from 10,000 years at 500 m and 8 years at 1 m depths. These calculations indicate that the transport process probably is slow.
- Upward moving saline groundwater may take place in the discharge areas. This means that it may be possible to induce a radionuclide transport into the biosphere. Rb, Th and Cs can together with Ca, SO_4 and Cl be indicators of deep water up flow. Correlation tests between Rb, Cs and Th and Cl, operational age and deep saline water were performed (in Appendix 3). A correlation is obtained at high Cl concentrations. At dilute waters and a depth of few meters there are no apparent correlations due to strong dilution or that the elements are affected by reactions. Some of the trace elements may have problems with the accuracy but a good internal correlation between the elements may indicate that these elements may not have a severe analytical problem. It is well known /e.g. Landström and Tullborg 1995/ that Rb, Th and Cs are generally absorbed on to the fracture minerals along the flow paths in addition slow ion exchange may lead to a non water conservative transport. These elements can also be transported in colloidal form (A Möri, pers comm. 2002). The calculated dilution effect indicated also that in average less than 2% of the original concentration at repository depth reaches the biosphere. This means that measured correlation with Cl may well be an

effect of input from several end-members in the same way as the Cl is modelled to have several sources. It is concluded that Cl, Ca, SO_4, Rb, Th and Cs can be useful tracers for the transport processes from the repository level to the biosphere but only a small fraction may be from the repository level.

For the future the isotopes of Rb, Cs, Cl and C could be analysed in order to test if these elements can indicate more conclusive deep water signatures. By using a more detailed hydrogeological modelling together with sampling campaign reflecting the spatial and temporal variations could give more information of the interaction between deep and shallow waters. Repeated analyses for some of the deep samples could indicate the accuracy of the trace element analyses. Repeated sampling could give information of the seasonal variability but also indications of sampling points with more constant hydrochemical conditions which may indicate influences from deep water. Colloidal transport of the elements is known to take place in the surface waters /Andersson et al. 2001, Artinger et al. 2002/. Therefore it could be of interest to filter the groundwater and analyse these filters in a future campaign. Noble gas analyses from various depths could be used to trace the deep input but this has to be combined with detailed modelling. An element or isotope ratio of an element cannot be used to indicate the deep origin without compensating for possible sources along the flow path.

8 Acknowledgements

This study has been supported and financed by the Swedish Nuclear and Waste Management Company (SKB). The helpful discussions and suggestions from Ulrik Kautsky (SKB) Peter Wikberg (SKB) and Ignasi Puigdomenech (SKB) are acknowledged. Helpful contributions and suggestions from Eva-Lena Tullborg (Terralogica AB) and Bill Wallin (Geokema AB) are acknowledged. Cecilia Andersson (INTERA) and Stefan Dahlgren (Dafoc) helped with the sampling and with the background information for some of the modelling and figures. Ann-Chatrin Nilsson (KTH) and Anna-Säfvestad (SKB) were in charge for the chemical analyses.

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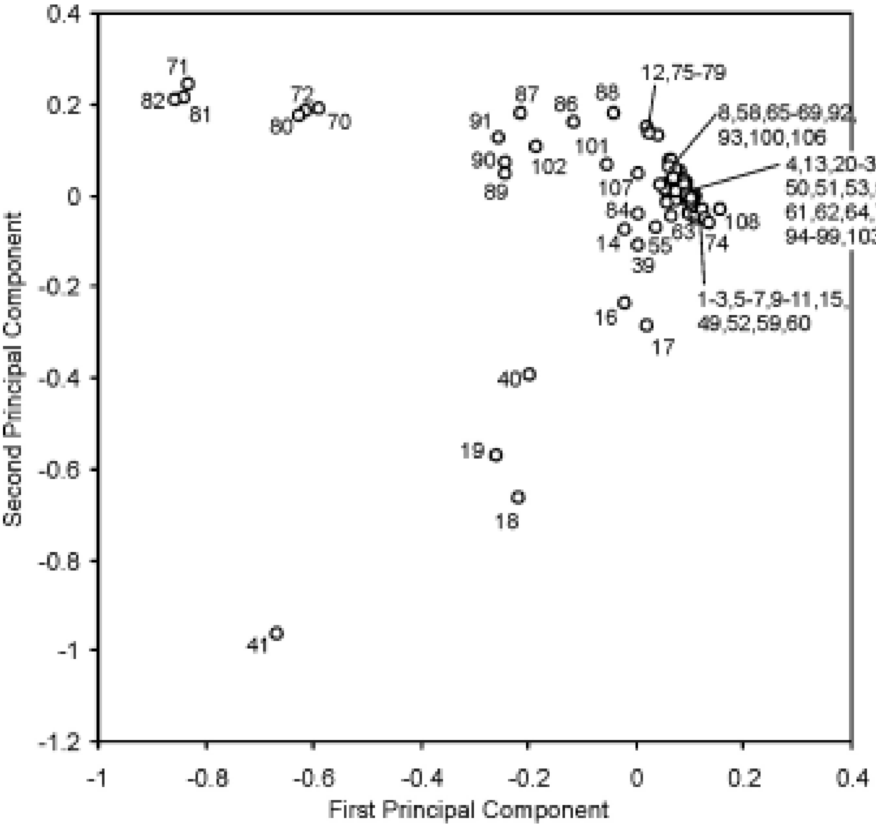
Appendix 1

Groundwater compositions; M3 modelling results and operational ages for 2 chosen models

For orientation the PCA-plot below (Figure A1-1) shows the observations as table row numbers. The analytical data have been extracted from the SKB database SICADA.



First Principal Component = – 0.42[Na] – 0.22[K] – 0.04[Ca] – 0.05[Mg]–
0.17[HCO_3] + 0.14[Cl] – 0.11[SO_4] – 0.06[O18] – 0.70[D] + 0.46[Tr]
Second Principal Component = – 0.42[Na] + 0.18[K] – 0.11[Ca] – 0.15[Mg]–
0.30[HCO_3] + 0.10[Cl] – 0.39[SO_4] – 0.60[O18] + 0.37[D] – 0.06[Tr]

Variance:
Component 1 = 48%
Component 1+2 = 73%

Figure A1-1. *Principal component plot based on the 108-sampled surface/shallow water data together with Laxemar data to a depth of 1,000 m. The variables analysed are Na, K, Ca, Mg, HCO3, Cl, SO4, $\delta^{18}O$, $\delta^{2}H$ and ^{3}H. The first and second principal components summarise 73% of the total information in the variables. The row numbers used in the analytical table listed in this appendix are indicated.*

The table in this appendix lists the following: row number, identification code for the boreholes, sample numbers, major components, stable isotopes, tritium, nitrate, phosphate, M3 mixing proportions, the deviation from the M3 mixing calculations for all the elements, calculated dilution of Cl from the depth of 500 m, distance to the sea and the operational age using two models where the age for the Baltic sea is varied from 0 to 3,000 years. The operational age represent a calculated mean residence time based on assumed ages for the reference waters and the mixing proportions for the observations.

The analytical values listed in the table are represented graphically (Figure A1-2) in this appendix as a multi-plot where the variables are plotted against each other in a series of scatter plots. The analytical data have been extracted from the SKB database SICADA.

Explanation of the footnotes and notations used in the table:

- –1.#ND indicates observations in the PCA outside the polygone and they are therefore not modelled.
- Italics SO4 = Calculated from SO4-S.
- Bold Tr = Estimated values: elevation 0: –800 m Tr = 22TU, elevation < –800 m Tr = 0TU.
- Underlined Mixing proportions = Estimated values for samples close to the polygon.
- Greyshaded rows = Samples within the modelled area.
- Marked cells: reference waters.
- SNO: sample number.

Row no.	Idcode (borehole)	SNO	Na mg/L 5%	K mg/L 5%	Ca mg/L 5%	Mg mg/L 5%	HCO3 mg/L 5%	Cl mg/L 5%	SO4 mg/L 10%	D SMOW 1 unit	O18 SMOW 0.2 unit	Tr TU 1 unit	NH4-N mg/L 20%	PO4-P mg/L 5%
1	HLX01	–1	32.5	2.2	37.8	4.9	115	18.1	47.8	–81	–10.9	34		
2	HLX01	–1	137	2.9	10.7	2.1	232	42.3	59.1	–79	–10.8	25		
3	HLX01	–1	141	3	11.5	1.9	233	40.9	63.8	–79	–10.9	17		
4	HLX02	2,562	4.3	0.72	7.4	1	31	–2.5	4.48	–75.9	–9.8	**22**		
5	HLX03	–1	76	5.1	15	3.9	210	11	21	–80	–10.8	25		
6	HLX03	–1	67	5	17	4.3	204	5.8	21.5	–80	–10.9	34		
7	HLX04	2,557	102	2.98	11.9	2.7	220	32	41.1	–80.9	–10.8	**22**		
8	HLX05	2,558	50.5	3.83	45.4	8.7	347	5.4	6.92	–74.4	–9.7	**22**		
9	HLX06	2,559	17.2	1.54	24.7	3.4	154	4.2	7.35	–78.6	–10.2	**22**		
10	HLX06	–1	56.1	2.8	24.5	4.9	219	5.7	8.7	–77	–10.6	17		
11	HLX06	–1	92	2	12.3	2.3	249	12.1	23.5	–77	–10.6	17		
12	HLX07	2,560	3	0.51	4.4	1.2	21	3	4.44	–66.8	–8.6	**22**		
13	HLX07	–1	170	5.2	27.5	6.1	151	215	72	–76	–10.5	25		
14	HLX07	–1	430	5.6	42	9.2	200	440	260	–78	–10.8	8.4		
15	HLX08	2,561	35.7	2.75	9.8	7.2	75	56.4	9	–80.7	–10.5	**22**		
16	KLX01	1,537	1,040	6.2	243	28	83	2,050	48	–89.9	–11.5	8	0.081	0.001
17	KLX01	1,528	860	6.1	223	18	78	1,700	106	–94.5	–12.2	8	0.061	0.003
18	KLX01	1,516	1,680	7.1	1,400	23	24	4,870	351	–102.1	–13.3	8	0.004	0.002
19	KLX01	1,633	1,610	7.3	1,330	24	24	4,680	390	–98.8	–11.8	8	0.04	0.003
20	KLX02	–1	137	3.9	54.1	4.4	220	149	*61.124*	–74.4	–9.9	8.4		
21	KLX02	–1	134	3.9	45.7	4.3	202	146	*58.127*	–75.1	–10.5	5.9		
22	KLX02	–1	130	3.8	43.4	4.3	200	140	*56.629*	–74.6	–10.7	4.2		
23	KLX02	–1	120	3.7	39.3	4.3	200	123	*52.434*	–76.3	–10.3	11.8		
24	KLX02	–1	110	4.3	38.6	4.3	202	109	*48.839*	–76.1	–10.4	15.2		
25	KLX02	–1	97.4	3.5	33.8	4.3	202	82.5	*43.745*	–76.3	–10.5	12.7		
26	KLX02	–1	87	3.5	31.5	4.3	205	63.8	*40.15*	–75.9	–10.5	5.1		
27	KLX02	–1	77	3.5	29.1	4.3	205	45	*36.554*	–75.4	–10.7	7.6		
28	KLX02	–1	72.9	3.4	27.4	4.5	205	34.5	*33.558*	–76.4	–10.7	7.6		

Row no.	**Idcode (borehole)**	**SNO**	**Na mg/L 5%**	**K mg/L 5%**	**Ca mg/L 5%**	**Mg mg/L 5%**	**HCO3 mg/L 5%**	**Cl mg/L 5%**	**SO4 mg/L 10%**	**D SMOW 1 unit**	**O18 SMOW 0.2 unit**	**Tr TU 1 unit**	**NH4-N mg/L 20%**	**PO4-P mg/L 5%**
29	KLX02	–1	69.5	3.4	26.2	4.6	204	28	*32.06*	–75.5	–10.6	8.4		
30	KLX02	–1	67.7	3.5	25.6	4.7	202	26.5	*31.161*	–76.2	–10.6	12.7		
31	KLX02	–1	67.3	3.5	25.3	4.7	198	26.2	*30.562*	–75.3	–10.6	16.1		
32	KLX02	–1	67.6	3.4	25.5	4.5	201	25.5	*29.783*	–76.5	–10.4	8.4		
33	KLX02	–1	67.4	3.4	25.3	4.5	200	28	*29.753*	–75.5	–10.4	8.4		
34	KLX02	–1	68.2	3.5	25.5	4.5	200	28.3	*29.843*	–76	–10.4	17.7		
35	KLX02	–1	67.6	3.4	25.9	4.5	209	28	*29.963*	–76.6	–10.5	19.4		
36	KLX02	–1	68.8	3.4	28.3	4.5	202	34	*31.161*	–75.5	–10.5	15.2		
37	KLX02	–1	73.4	3.4	38.9	4.3	205	60	*35.356*	–75.1	–10.7	12.7		
38	KLX02	–1	103	3.4	82.6	4.5	202	175	*48.24*	–76.1	–10.4	11		
39	KLX02	–1	327	3.7	397	4.6	181	1,080	*125.54*	–77.8	–10.7	13.5		
40	KLX02	–1	1,000	5.1	1,340	4.7	126	3,780	*302.62*	–81.5	–11.3	11		
41	KLX02	–1	2,460	8.5	3,590	4	53	9,910	*644.2*	–84.5	–11.9	10.1		
42	KLX02	2,406	61	4.05	29.2	5.9	0	150.1	3.68	–76.5	–9.5	**22**		
43	KLX02	2,413	62.6	3.8	33.6	6	51	119.6	4.04	–77.4	–9.7	**22**		
44	KLX02	2,416	53.6	3.3	34.4	6.9	182	46	9.41	–77.4	–10	6		
45	KLX02	2,421	50.8	4.9	37.2	7.4	205	36.1	12.19	–77.7	–10	**22**		
46	KLX02	2,422	58	3.75	32.1	6.5	139	65.8	6.41	–77	–9.9	**22**		
47	KLX02	2,424	52	3.05	39.6	7.7	209	35.4	12.77	–77.8	–10	10		–0.14
48	KLX02	2,412	57.5	3.2	53.4	7.4	217	83.4	14.76	–79.3	–10	**0**		
49	KLX02	2,418	50.3	3.2	38.1	7.4	215	35.4	13.26	–82.2	–10	**0**		
50	KLX02	2,419	50.4	4.8	39.1	7.6	213	34.7	12.92	–79.3	–10	**0**		
51	KLX02	2,420	51.2	4.25	39.4	7.6	212	35.4	13.67	–78.1	–10	**22**		
52	KLX02	2,427	51.6	3.1	40.1	7.8	212	35.4	13.06	–81.2	–10.1	10		
53	KLX02	2,705	206	3.1	36	5.9	201	235	84	–75.7	–10.6	**22**		
54	KLX02	2,738	111	3.1	24	4.6	223	73	43	–73.4	–10.3	**22**	0.1	0.03
55	KLX02	2,712	288	4.5	123	10.6	111	548	105	–78.7	–10.9	**22**	0.07	–0.01

Row no.	Idcode (borehole)	SNO	Na mg/L 5%	K mg/L 5%	Ca mg/L 5%	Mg mg/L 5%	HCO3 mg/L 5%	Cl mg/L 5%	SO4 mg/L 10%	D SMOW 1 unit	O18 SMOW 0.2 unit	Tr TU 1 unit	NH4-N mg/L 20%	PO4-P mg/L 5%
56	PLX00013	2,523	8.5	1.3	29.6	4.8	84	10.8	24	–77.2	–10	**22**		
57	PLX00014	2,524	9	2.43	36.1	5.3	109	11.1	29.2	–76.3	–9.9	**22**		
58	PLX00015	2,526	9.3	1.72	11	2.6	25	11.8	13	–73.8	–9.2	**22**		
59	PLX00017	2,528	4.4	0.85	4.2	1.2	9	6.6	4.88	–80.6	–10.5	**22**		
60	PLX00018	2,529	4.6	1.23	5.2	1.6	7	6.1	12.4	–82.4	–10.7	**22**		
61	PLX00020	2,531	2.9	1.3	3.8	0.8	9	3.8	5.78	–79.8	–10	**22**		
62	PLX00021	2,532	31.6	4.61	19.2	6	84	53.2	19.3	–78.5	–9.8	**22**		
63	PLX00022	2,533	202	4.19	37.8	16	228	259	83.7	–81	–10.6	**22**		
64	PLX00023	3,031	10.8	2.48	11.4	2.8	28	10.2	*17.318*	–75.7	–9.9	13.6		
65	PLX00023	2,534	9.1	1.64	11.5	2.6	25	18.6	13.03	–72.7	–9.3	**22**	–	0.03
66	PLX00024	2,535	9	1.52	11.4	2.5	27	17.3	11.7	–73.9	–9.7	**22**		
67	PLX00025	2,536	9	1.54	11.4	2.5	25	16.9	12	–71.6	–9.2	**22**		
68	PLX00026	2,537	9.1	1.49	11.4	2.6	25	17.5	12.8	–74.4	–9.4	**22**		
69	PLX00027	2,538	9	1.48	11.4	2.6	25	12.9	12.4	–73.9	–9.4	**22**		
70	PLX00030	2,541	1,400	51.7	64.7	180	68	2,820	353	–59.8	–7.2	**22**		
71	PLX00031	3,016	1,920	74.9	92.2	236	93	3,510	*479.4*	–56.4	–6.1	17.2		
72	PLX00031	2,542	1,410	51.3	64.7	178	68	3,150	388	–57.8	–7.2	**22**	–	0.012
73	PLX00032	2,543	40	2.57	26.7	16.3	234	13.5	7.78	–78.6	–10.3	**22**		
74	PLX00033	2,544	4.2	1.28	7.3	1.9	12	15.1	4.56	–83.9	–10.8	**22**		
75	PLX00034	2,545	13	1.7	8.7	2.8	16	24.2	20.5	–68.6	–8	**22**		
76	PLX00035	2,546	12.6	1.83	8.7	2.8	17	24.2	17.9	–68.5	–8.1	**22**		
77	PLX00036	2,547	12.5	1.85	9.1	2.9	20	21.1	16.3	–67.8	–8.2	**22**		
78	PLX00037	2,548	13	1.85	9.1	3	20	23.2	15.9	–66.9	–8.1	**22**		
79	PLX00038	2,549	27.2	2.51	9.3	4.7	26	44.6	19.7	–69.3	–8.1	**22**		
80	PLX00039	2,550	1,460	54	66.7	186	71	3,200	394	–60.3	–7.1	**22**		
81	PLX00040	3,017	1,970	75.1	94.1	242	95	3,670	*503.37*	–57.5	–6.5	17.8		
82	PLX00040	2,551	1,930	70.1	83.8	249	91	4,300	530	–56.5	–6.4	**22**	–	0.018

Row no.	**Idcode (borehole)**	**SNO**	**Na mg/L 5%**	**K mg/L 5%**	**Ca mg/L 5%**	**Mg mg/L 5%**	**HCO3 mg/L 5%**	**Cl mg/L 5%**	**SO4 mg/L 10%**	**D SMOW 1 unit**	**O18 SMOW 0.2 unit**	**Tr TU 1 unit**	**NH4-N mg/L 20%**	**PO4-P mg/L 5%**
83	PLX00041	2,552	9.1	3.04	14.5	3.7	30	26.3	16.6	–77.4	–10.1	**22**		
84	PLX00042	2,553	420	13.5	45.9	23.3	202	493	86.2	–80.5	–10.5	**22**		
85	PLX00043	2,554	10	2.97	16	3.5	24	22.1	35.7	–77.2	–10.1	**22**		
86	PLX00044	3,010	101	3.38	106	35	–8	267	*225.02*	–62.9	–7.6	15.4	–	x
87	PLX00045	3,011	447	10.8	140	63.1	–11	1,060	*189.06*	–59.9	–7.3	15.4	–	x
88	PLX00046	3,012	143	10.6	36	35.7	290	234	*12.884*	–66.1	–7.9	15.1	–	x
89	PLX00047	3,013	585	21	82.3	111	276	950	*353.56*	–72.1	–9.3	16	–	x
90	PLX00048	3,014	757	27.2	76.3	107	518	1,360	*237.3*	–71.2	–9.1	17.1	–	0.241
91	PLX00049	3,015	813	36	72.1	101	471	1,450	*125.24*	–68.3	–8.6	12.1	–	x
92	PLX00050	3,018	24.9	1.44	17	12	152	16.8	*7.4906*	–73	–9.2	13.9	–	0.041
93	PLX00051	3,019	39.6	0.7	30	11.8	171	32	*33.858*	–73.3	–9.4	14.2	–	x
94	PLX00052	3,020	63.5	6.08	31.1	20.9	329	31.8	*11.116*	–77.6	–10	13.1	–	0.118
95	PLX00053	3,021	176	7.96	51.4	52	616	166	*9.0787*	–80.4	–10.3	12.8	–	x
96	PLX00054	3,022	169	8.46	45.9	37.4	406	221	*7.7903*	–79	–10.1	13.4	–	x
97	PLX00055	3,023	9.3	1.5	10.8	2.5	53	9.7	*8.1798*	–76.2	–9.7	14.5	–	x
98	PLX00056	3,024	12.9	1.05	9.1	3.3	51	11.9	*8.2697*	–76	–9.9	14.2	–	x
99	PLX00057	3,025	39.3	1.93	15.2	13.6	163	33.4	*8.4794*	–77.4	–9.9	21.6	–	x
100	PLX00058	3,026	65.6	5.35	16.8	19	212	60.4	*5.633*	–76.6	–9.8	13.6	–	x
101	PLX00059	3,027	318	13.5	28.8	42.8	–6	471	*65.318*	–72	–9.4	15.8	–	0.053
102	PLX00060	3,028	565	20.6	47.1	77.2	93	900	*163.6*	–68.6	–8.6	14.2	–	0.02
103	PLX00061	3,029	139	2.04	24.4	20.6	156	244	*5.0337*	–77.4	–10.1	15.3	–	x
104	PLX00062	3,030	44.8	2	18.1	16.3	179	39	*14.442*	–77.9	–10.3	16.4	–	x
105	PLX00063	3,032	33.3	3.21	16.2	6.2	103	33.6	*1.8277*	–80	–10.1	14	–	x
106	PLX00064	3,033	137.5	6.88	21.3	27.2	177	219	*25.228*	–76.3	–10	14.8	–	x
107	PLX00065	3,034	269	15.4	29.8	38.5	426	376	*16.629*	–75.2	–9.9	10.5	–	x
108	Rain’60		0.4	0.29	0.24	0.1	12.2	0.23	1.41	–80	–10.5	2,000		

Cont.

Row no.	Idcode (borehole)	SNO	Date	Northing RT (coordinates)	Easting RT (coordinates)	Elevation RT (depth below sea level)	Comment	Reference water	Baltic Sea Mixing Proportion	Surface Mixing Proportion	Meteoric Mixing Proportion	Deep Saline Mixing Proportion
1	HLX01	–1	871023	6367316.702	1549572.966	–56.577	Borehole		3%	3%	82%	13%
2	HLX01	–1	871024	6367316.702	1549572.966	–56.577	Borehole		4%	4%	82%	9%
3	HLX01	–1	871025	6367316.702	1549572.966	–56.577	Borehole		4%	4%	81%	10%
4	HLX02	2,562	980617 04:00:00	6368102.13	1549936.269	–8.106	Borehole		2%	33%	64%	2%
5	HLX03	–1	871105	6367794.515	1549919.097	–46.697	Borehole		4%	4%	87%	6%
6	HLX03	–1	871106	6367794.515	1549919.097	–46.697	Borehole		3%	3%	87%	7%
7	HLX04	2,557	980617 04:00:00	6367683.3	1549788.515	–7.483	Borehole		3%	3%	84%	10%
8	HLX05	2,558	980617 04:00:00	6367547.897	1549969.599	–1.466	Borehole		1%	45%	52%	1%
9	HLX06	2,559	980617 04:00:00	6367155.622	1549784.187	–1.126	Borehole		2%	16%	79%	2%
10	HLX06	–1	871101	6367128.243	1549781.304	–46.41	Borehole		3%	15%	80%	3%
11	HLX06	–1	871103	6367128.243	1549781.304	–46.41	Borehole		3%	13%	81%	3%
12	HLX07	2,560	980617 04:00:00	6367158.346	1550021.322	–8.434	Borehole		0%	13%	87%	0%
13	HLX07	–1	871104	6367169.252	1550035.626	–44.711	Borehole		8%	10%	74%	8%
14	HLX07	–1	871105	6367169.252	1550035.626	–44.711	Borehole		11%	11%	41%	37%
15	HLX08	2,561	980617 04:00:00	6366585.403	1550591.414	–2.358	Borehole		4%	4%	88%	5%
16	KLX01	1,537	881208	6367503.796	1549918.294	–257.015	Borehole		6%	3%	3%	89%
17	KLX01	1,528	881123	6367514.415	1549916.074	–440.693	Borehole	Deep Saline	0%	0%	0%	100%
18	KLX01	1,516	881103	6367526.807	1549914.193	–672.907	Borehole		–1.#IND	–1.#IND	–1.#IND	–1.#IND
19	KLX01	1,633	891101	6367526.807	1549914.193	–672.907	Borehole		–1.#IND	–1.#IND	–1.#IND	–1.#IND
20	KLX02	–1	930803	6366770.339	1549224.151	–1.614	Borehole		6%	29%	59%	6%
21	KLX02	–1	930803	6366773.535	1549224	–37.471	Borehole		6%	15%	73%	6%
22	KLX02	–1	930803	6366778.22	1549223.779	–87.251	Borehole		6%	13%	75%	6%
23	KLX02	–1	930803	6366782.71	1549223.567	–137.048	Borehole		6%	16%	73%	6%
24	KLX02	–1	930803	6366787.157	1549223.357	–186.85	Borehole		5%	16%	73%	5%
25	KLX02	–1	930803	6366791.58	1549223.1	–236.653	Borehole		5%	14%	76%	5%

Row no.	Idcode (borehole)	SNO	Date	Northing RT (coordinates)	Easting RT (coordinates)	Elevation RT (depth below sea level)	Comment	Reference water	Baltic Sea Mixing Proportion	Surface Mixing Proportion	Meteoric Mixing Proportion	Deep Saline Mixing Proportion
26	KLX02	–1	930803	6366796.014	1549222.896	–286.455	Borehole		4%	16%	75%	4%
27	KLX02	–1	930803	6366800.646	1549222.65	–336.24	Borehole		4%	15%	77%	4%
28	KLX02	–1	930803	6366805.77	1549222.479	–385.976	Borehole		4%	12%	80%	4%
29	KLX02	–1	930803	6366811.098	1549222.401	–435.691	Borehole		4%	18%	75%	4%
30	KLX02	–1	930803	6366816.632	1549222.264	–485.384	Borehole		4%	15%	77%	4%
31	KLX02	–1	930803	6366822.335	1549222.126	–535.057	Borehole		4%	19%	74%	4%
32	KLX02	–1	930803	6366828.089	1549222.149	–584.725	Borehole		4%	18%	74%	4%
33	KLX02	–1	930803	6366833.836	1549222.179	–634.393	Borehole		4%	22%	71%	4%
34	KLX02	–1	930803	6366839.809	1549222.204	–684.035	Borehole		4%	20%	73%	4%
35	KLX02	–1	930803	6366845.776	1549222.199	–733.678	Borehole		4%	16%	77%	4%
36	KLX02	–1	930803	6366851.627	1549222.224	–783.334	Borehole		4%	19%	73%	4%
37	KLX02	–1	930803	6366857.641	1549222.186	–832.971	Borehole		4%	15%	76%	4%
38	KLX02	–1	930803	6366863.646	1549221.955	–882.609	Borehole		6%	12%	77%	6%
39	KLX02	–1	930803	6366869.595	1549221.565	–932.252	Borehole		8%	8%	38%	46%
40	KLX02	–1	930803	6366875.635	1549221.34	–981.885	Borehole		–1.#IND	–1.#IND	–1.#IND	–1.#IND
41	KLX02	–1	930803	6366881.728	1549221.359	–1,031.513	Borehole		–1.#IND	–1.#IND	–1.#IND	–1.#IND
42	KLX02	2,406	970925 10:00:00	6366770.774	1549224.13	–6.595	Borehole		4%	34%	58%	4%
43	KLX02	2,413	970925 10:00:00	6366779.909	1549223.699	–106.175	Borehole		4%	28%	64%	4%
44	KLX02	2,416	970925 10:00:00	6366797.73	1549222.8	–305.377	Borehole		3%	25%	69%	3%
45	KLX02	2,421	970925 10:00:00	6366807.777	1549222.442	–404.87	Borehole		3%	25%	69%	3%
46	KLX02	2,422	970925 10:00:00	6366788.811	1549223.276	–205.777	Borehole		3%	27%	66%	3%
47	KLX02	2,424	970925 10:00:00	6366818.786	1549222.2	–504.261	Borehole		3%	23%	71%	3%
48	KLX02	2,412	970925 10:00:00	6366877.951	1549221.322	–1,000.744	Borehole		4%	16%	76%	4%
49	KLX02	2,418	970925 10:00:00	6366865.92	1549221.818	–901.472	Borehole		4%	7%	85%	4%
50	KLX02	2,419	970925 10:00:00	6366853.89	1549222.216	–802.199	Borehole		4%	19%	74%	4%
51	KLX02	2,420	970925 10:00:00	6366830.244	1549222.16	–603.602	Borehole		3%	23%	71%	3%
52	KLX02	2,427	970925 10:00:00	6366842.08	1549222.196	–702.899	Borehole		4%	9%	84%	4%

Row no.	Idcode (borehole)	SNO	Date	Northing RT (coordinates)	Easting RT (coordinates)	Elevation RT (depth below sea level)	Comment	Reference water	Baltic Sea Mixing Proportion	Surface Mixing Proportion	Meteoric Mixing Proportion	Deep Saline Mixing Proportion
53	KLX02	2,705	931108	6366798.92	1549222.733	–318.222	Borehole		8%	8%	76%	9%
54	KLX02	2,738	940210	6366797.112	1549222.834	–298.656	Borehole		4%	29%	63%	4%
55	KLX02	2,712	931123	6366851.023	1549222.226	–778.27	Borehole		7%	7%	56%	29%
56	PLX00013	2,523	980602 04:00:00	6367010	1547440	12	Ditch		3%	23%	71%	3%
57	PLX00014	2,524	980602 04:00:00	6367470	1547540	12	Ditch		3%	28%	65%	3%
58	PLX00015	2,526	980603 04:00:00	6370250	1548100	3	Ditch		2%	52%	44%	2%
59	PLX00017	2,528	980603 04:00:00	6369320	1548150	9.5	Digged well		3%	3%	91%	4%
60	PLX00018	2,529	980603 04:00:00	6369980	1547920	12	Spring		2%	2%	87%	10%
61	PLX00020	2,531	980603 04:00:00	6370950	1546600	13	Spring		3%	15%	80%	3%
62	PLX00021	2,532	980603 04:00:00	6368990	1548800	5	Digged well		4%	24%	68%	4%
63	PLX00022	2,533	980603 04:00:00	6369020	1548720	–33	Drilled well		6%	6%	70%	17%
64	PLX00023	3,031	991014	6369150	1548850	5	Ditch		3%	31%	63%	3%
65	PLX00023	2,534	980604 04:00:00	6369150	1548850	5	Ditch		2%	54%	43%	2%
66	PLX00024	2,535	980604 04:00:00	6369070	1548890	0	Ditch		2%	42%	55%	2%
67	PLX00025	2,536	980604 04:00:00	6369040	1548920	0	Ditch		1%	60%	37%	1%
68	PLX00026	2,537	980604 04:00:00	6369020	1548960	0	Ditch		2%	46%	50%	2%
69	PLX00027	2,538	980604 04:00:00	6369030	1549000	0	Ditch		2%	48%	49%	2%
70	PLX00030	2,541	980604 04:00:00	6368710	1550040	0	Baltic Sea		72%	18%	5%	5%
71	PLX00031	3,016	991012	6368840	1549630	0	Baltic Sea	Baltic Sea	100%	0%	0%	0%
72	PLX00031	2,542	980604 04:00:00	6368840	1549630	0	Baltic Sea		75%	13%	6%	6%
73	PLX00032	2,543	980604 04:00:00	6368800	1549450	–35	Drilled well		3%	18%	76%	3%
74	PLX00033	2,544	980604 04:00:00	6368790	1549440	3	Digged well		0%	0%	87%	12%
75	PLX00034	2,545	980605 04:00:00	6368280	1549450	3	Lake		0%	95%	4%	0%
76	PLX00035	2,546	980605 04:00:00	6368330	1549710	2	Ditch		0%	94%	5%	0%
77	PLX00036	2,547	980605 04:00:00	6368470	1550020	0	Ditch		0%	95%	5%	0%
78	PLX00037	2,548	980605 04:00:00	6368470	1550060	0	Ditch	Surface	0%	100%	0%	0%
79	PLX00038	2,549	980605 04:00:00	6368470	1550100	0	Ditch		1%	91%	7%	1%

Row no.	Idcode (borehole)	SNO	Date	Northing RT (coordinates)	Easting RT (coordinates)	Elevation RT (depth below sea level)	Comment	Reference water	Baltic Sea Mixing Proportion	Surface Mixing Proportion	Meteoric Mixing Proportion	Deep Saline Mixing Proportion
80	PLX00039	2,550	980605 04:00:00	6368490	1550170	0	Baltic Sea		77%	7%	7%	8%
81	PLX00040	3,017	991012	6369600	1555200	0	Baltic Sea		–1.#IND	–1.#IND	–1.#IND	–1.#IND
82	PLX00040	2,551	980605 04:00:00	6369600	1555200	0	Baltic Sea		–1.#IND	–1.#IND	–1.#IND	–1.#IND
83	PLX00041	2,552	980615 04:00:00	6370400	1547600	5	Gravel–pit		3%	21%	72%	3%
84	PLX00042	2,553	980615 04:00:00	6370300	1547650	–35	Drilled well		11%	11%	54%	24%
85	PLX00043	2,554	980615 04:00:00	6368930	1549380	0	Ditch		4%	20%	72%	4%
86	PLX00044	3,010	991012	6368462	1550042	–0.57	Soil tube		16%	82%	1%	1%
87	PLX00045	3,011	991012	6368464	1550051	–0.66	Soil tube		28%	72%	0%	0%
88	PLX00046	3,012	991012	6368469	1550066	–1.5	Soil tube		9%	91%	0%	0%
89	PLX00047	3,013	991012	6368498	1550065	–1.05	Soil tube		35%	21%	21%	22%
90	PLX00048	3,014	991012	6368511	1550057	–1.2	Soil tube		34%	30%	18%	18%
91	PLX00049	3,015	991012	6368516	1550054	–1.23	Soil tube		34%	48%	9%	9%
92	PLX00050	3,018	991013	6369097	1549074	–0.57	Soil tube		1%	59%	39%	1%
93	PLX00051	3,019	991013	6369095	1549077	–0.7	Soil tube		2%	50%	45%	2%
94	PLX00052	3,020	991013	6369095	1549078	–1.55	Soil tube		3%	31%	62%	3%
95	PLX00053	3,021	991013	6369083	1549084	–3.47	Soil tube		6%	22%	67%	6%
96	PLX00054	3,022	991013	6369087	1549044	–3.81	Soil tube		6%	24%	63%	6%
97	PLX00055	3,023	991013	6369078	1548932	–0.7	Soil tube		2%	34%	62%	2%
98	PLX00056	3,024	991013	6369078	1548937	–1.01	Soil tube		2%	30%	65%	2%
99	PLX00057	3,025	991013	6369075	1548939	–2.18	Soil tube		3%	29%	66%	3%
100	PLX00058	3,026	991013	6369076	1548952	–4.13	Soil tube		3%	37%	56%	3%
101	PLX00059	3,027	991014	6368982	1549218	–0.375	Soil tube		13%	52%	23%	13%
102	PLX00060	3,028	991014	6368985	1549219	–0.55	Soil tube		26%	52%	11%	11%
103	PLX00061	3,029	991014	6368992	1549222	–1.58	Soil tube		5%	20%	70%	5%
104	PLX00062	3,030	991014	6368977	1548961	–2.2	Soil tube		3%	19%	75%	3%
105	PLX00063	3,032	991014	6369010	1549173	–0.9	Soil tube		3%	14%	80%	3%
106	PLX00064	3,033	991014	6369013	1549176	–2.17	Soil tube		6%	30%	57%	6%
107	PLX00065	3,034	991014	6369081	1549120	–3.95	Soil tube		8%	43%	40%	8%
108	Rain'60							Meteroic	0%	0%	100%	0%

Cont.

Row no.	Idcode (borehole)	SNO	Na mg/L Deviation	K mg/L Deviation	Ca mg/L Deviation	Mg mg/L Deviation	HCO3 mg/L Deviation	Cl mg/L Deviation	SO4 mg/L Deviation	D dev SMOW Deviation	O18 dev SMOW Deviation	Tr TU Deviation	Dilution of Cl in % from 500 m
1	HLX01	–1	–125	–1	7	–4	92	–285	21	0	0	–1,616	0.13%
2	HLX01	–1	–23	–1	–14	–10	210	–261	27	1	0	–1,627	0.22%
3	HLX01	–1	–28	–1	–16	–10	210	–281	31	1	–1	–1,614	0.25%
4	HLX02	2,562	–46	–1	–1	–4	14	–97	–11	0	0	–1,266	0.00%
5	HLX03	–1	–45	2	–2	–6	191	–218	–4	0	0	–1,713	0.04%
6	HLX03	–1	–55	2	–2	–5	184	–226	–3	0	–1	–1,700	0.02%
7	HLX04	2,557	–41	0	–13	–6	199	–242	15	–1	0	–1,662	0.19%
8	HLX05	2,558	6	2	37	4	329	–78	–9	0	0	–1,029	0.00%
9	HLX06	2,559	–51	–1	16	–3	137	–123	–10	–1	0	–1,569	0.01%
10	HLX06	–1	–22	0	14	–3	202	–140	–11	1	–1	–1,586	0.01%
11	HLX06	–1	4	–1	1	–6	231	–152	2	1	0	–1,606	0.02%
12	HLX07	2,560	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	0.00%
13	HLX07	–1	–46	–1	2	–14	127	–190	24	2	0	–1,463	0.98%
14	HLX07	–1	–105	–5	–52	–24	154	–586	165	3	0	–810	9.57%
15	HLX08	2,561	–77	–1	–5	–3	56	–156	–16	–1	0	–1,736	0.16%
16	KLX01	1,537	171	–3	40	–1	8	349	–73	1	0	–59	106.91%
17	KLX01	1,528	0	0	0	0	0	0	0	0	0	0	100.00%
18	KLX01	1,516	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
19	KLX01	1,633	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
20	KLX02	–1	–25	–1	33	–11	197	–154	22	1	0	–1,186	0.50%
21	KLX02	–1	–37	–2	25	–12	180	–174	19	2	–1	–1,459	0.52%
22	KLX02	–1	–38	–1	23	–11	178	–174	19	3	–1	–1,504	0.49%
23	KLX02	–1	–37	–1	20	–10	178	–171	16	1	0	–1,449	0.40%
24	KLX02	–1	–42	–1	20	–10	181	–176	14	1	0	–1,457	0.35%
25	KLX02	–1	–40	–1	17	–9	182	–175	12	1	0	–1,518	0.24%
26	KLX02	–1	–40	–1	16	–8	185	–173	10	2	–1	–1,494	0.17%

Row no.	Idcode (borehole)	SNO	Na mg/L Deviation	K mg/L Deviation	Ca mg/L Deviation	Mg mg/L Deviation	HCO3 mg/L Deviation	Cl mg/L Deviation	SO4 mg/L Deviation	D dev SMOW Deviation	O18 dev SMOW Deviation	Tr TU Deviation	Dilution of Cl in % from 500 m
27	KLX02	–1	–41	0	14	–7	186	–176	9	2	–1	–1,531	0.11%
28	KLX02	–1	–43	0	13	–6	186	–183	6	2	–1	–1,593	0.08%
29	KLX02	–1	–38	0	12	–6	185	–173	6	2	–1	–1,493	0.06%
30	KLX02	–1	–42	0	12	–6	183	–178	5	1	–1	–1,531	0.06%
31	KLX02	–1	–38	0	12	–5	179	–171	5	2	–1	–1,470	0.06%
32	KLX02	–1	–38	0	12	–6	182	–172	4	1	0	–1,481	0.06%
33	KLX02	–1	–34	0	12	–5	181	–162	5	1	–1	–1,416	0.06%
34	KLX02	–1	–36	0	12	–5	181	–167	4	1	0	–1,439	0.06%
35	KLX02	–1	–39	0	12	–6	190	–171	4	1	0	–1,516	0.06%
36	KLX02	–1	–37	0	15	–6	183	–165	5	2	–1	–1,452	0.07%
37	KLX02	–1	–46	–1	24	–7	185	–163	7	3	–1	–1,519	0.15%
38	KLX02	–1	–65	–2	63	–11	180	–139	10	2	0	–1,524	0.61%
39	KLX02	–1	–224	–5	286	–23	131	15	37	6	0	–752	29.32%
40	KLX02	–1	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
41	KLX02	–1	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
42	KLX02	2,406	–53	0	14	–5	–21	–63	–26	–1	0	–1,140	0.35%
43	KLX02	2,413	–48	0	19	–5	31	–87	–24	–1	0	–1,275	0.27%
44	KLX02	2,416	–35	0	22	–2	163	–120	–13	–1	0	–1,387	0.08%
45	KLX02	2,421	–45	2	24	–2	186	–143	–12	–1	0	–1,356	0.07%
46	KLX02	2,422	–35	0	19	–3	120	–108	–18	–1	0	–1,307	0.12%
47	KLX02	2,424	–37	0	28	–1	190	–131	–10	–1	0	–1,410	0.06%
48	KLX02	2,412	–51	0	40	–3	198	–119	–11	–2	0	–15,33	0.19%
49	KLX02	2,418	–56	0	25	–3	197	–164	–11	–4	0	–1,701	0.08%
50	KLX02	2,419	–52	1	26	–2	194	–157	–12	–2	0	–1,482	0.07%
51	KLX02	2,420	–45	1	27	–2	193	–143	–10	–1	0	–1,395	0.07%
52	KLX02	2,427	–53	0	27	–2	194	–161	–11	–3	0	–1,668	0.08%
53	KLX02	2,705	–20	–4	8	–14	176	–190	35	3	0	–1,495	1.22%
54	KLX02	2,738	–5	–1	8	–7	203	–144	14	2	–1	–1,239	0.17%

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55	KLX02	2,712	–102	–3	50	–12	73	–201	38	3	0	–1,113	9.42%
56	PLX00013	2,523	–80	–2	18	–4	66	–154	2	0	0	–1,409	0.02%
57	PLX00014	2,524	–83	–1	23	–4	90	–161	5	0	0	–1,290	0.02%
58	PLX00015	2,526	–43	–1	1	–3	6	–86	–6	–1	0	–875	0.01%
59	PLX00017	2,528	–82	–2	–8	–6	–8	–157	–14	–1	0	–1,792	0.02%
60	PLX00018	2,529	–107	–1	–18	–4	–13	–210	–6	–2	0	–1,728	0.03%
61	PLX00020	2,531	–73	–1	–6	–6	–8	–139	–13	–2	0	–1,585	0.01%
62	PLX00021	2,532	–78	1	5	–5	64	–152	–8	–2	0	–1,342	0.12%
63	PLX00022	2,533	–67	–2	–7	–2	199	–254	34	–1	0	–1,388	2.65%
64	PLX00023	3,031	–70	–1	0	–5	9	–140	–5	0	0	–1,259	0.02%
65	PLX00023	2,534	–41	–1	2	–3	6	–75	–5	0	0	–845	0.02%
66	PLX00024	2,535	–50	–1	1	–4	9	–93	–7	0	0	–1,079	0.02%
67	PLX00025	2,536	–33	–1	2	–2	6	–62	–5	0	0	–738	0.01%
68	PLX00026	2,537	–49	–1	1	–4	6	–90	–6	–1	0	–997	0.02%
69	PLX00027	2,538	–46	–1	1	–3	7	–89	–6	0	0	–964	0.01%
70	PLX00030	2,541	–36	–3	–15	8	–7	189	–2	2	0	–95	
71	PLX00031	3,016	0	0	0	0	0	0	0	0	0	0	
72	PLX00031	2,542	–86	–6	–19	–1	–10	408	19	3	0	–107	
73	PLX00032	2,543	–46	0	15	8	216	–148	–14	–1	0	–1,507	0.02%
74	PLX00033	2,544	–111	0	–21	–1	–9	–211	–12	–2	0	–1,714	0.11%
75	PLX00034	2,545	–10	0	–1	–1	–4	–17	3	–1	0	–76	0.01%
76	PLX00035	2,546	–9	0	–1	–1	–3	–15	1	–1	0	–105	0.00%
77	PLX00036	2,547	–6	0	0	0	0	–12	0	0	0	–97	0.00%
78	PLX00037	2,548	0	0	0	0	0	0	0	0	0	0	0.00%
79	PLX00038	2,549	–10	0	–2	0	5	–24	0	–1	0	–136	0.02%
80	PLX00039	2,550	–93	–5	–22	2	–9	351	14	2	0	–143	
81	PLX00040	3,017	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
82	PLX00040	2,551	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	

Row no.	Idcode (borehole)	SNO	Na mg/L Deviation	K mg/L Deviation	Ca mg/L Deviation	Mg mg/L Deviation	HCO3 mg/L Deviation	Cl mg/L Deviation	SO4 mg/L Deviation	D dev SMOW Deviation	O18 dev SMOW Deviation	Tr TU Deviation	Dilution of Cl in % from 500 m
83	PLX00041	2,552	–86	0	2	–5	11	–152	–7	0	0	–1,427	0.05%
84	PLX00042	2,553	5	4	–19	–7	164	–296	7	–1	0	–1,073	6.96%
85	PLX00043	2,554	–105	–1	1	–7	4	–193	8	0	0	–1,418	0.05%
86	PLX00044	3,010	–228	–10	82	–6	–40	–335	133	3	0	–21	0.12%
87	PLX00045	3,011	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
88	PLX00046	3,012	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	–1.#IND	
89	PLX00047	3,013	–276	–7	–1	24	219	–653	160	0	0	–426	12.45%
90	PLX00048	3,014	–52	0	2	23	464	–141	51	–1	–1	–355	14.32%
91	PLX00049	3,015	78	9	16	18	422	95	–55	–1	–1	–185	7.69%
92	PLX00050	3,018	–16	–1	8	7	133	–59	–9	–1	0	–774	0.01%
93	PLX00051	3,019	–36	–2	18	4	151	–109	11	0	0	–898	0.05%
94	PLX00052	3,020	–34	3	18	11	309	–151	–14	–2	0	–1,237	0.06%
95	PLX00053	3,021	10	3	31	36	594	–145	–30	–4	0	–1,325	0.57%
96	PLX00054	3,022	–7	3	24	21	383	–109	–33	–3	0	–1,256	0.81%
97	PLX00055	3,023	–51	–1	1	–4	35	–102	–10	–1	0	–1,232	0.01%
98	PLX00056	3,024	–50	–1	0	–3	33	–105	–10	0	0	–1,299	0.01%
99	PLX00057	3,025	–40	–1	4	6	145	–114	–13	–1	0	–1,303	0.05%
100	PLX00058	3,026	–31	2	3	9	192	–121	–20	–2	0	–1,123	0.12%
101	PLX00059	3,027	–37	2	–15	9	–41	–194	–17	0	0	–466	3.47%
102	PLX00060	3,028	–38	–1	–6	12	48	–216	18	0	0	–222	5.81%
103	PLX00061	3,029	–4	–3	6	7	135	–24	–29	–1	0	–1,383	0.72%
104	PLX00062	3,030	–53	–1	5	7	160	–144	–10	–1	0	–1,479	0.08%
105	PLX00063	3,032	–58	0	5	–2	85	–137	–20	–2	0	–1,582	0.06%
106	PLX00064	3,033	–44	1	–2	10	153	–120	–18	–1	0	–1,131	0.82%
107	PLX00065	3,034	32	8	0	16	398	–67	–39	–2	–1	–802	1.84%
108	Rain’60		0	0	0	0	0	0	0	0	0	0	

Cont.

Row no.	Idcode (borehole)	SNO	Dist to the sea m	Operational age model#1 = Baltic = 3,000; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS	Operational age model#2 = Baltic = 0; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS
1	HLX01	–1	802.0	1,377	1,300
2	HLX01	–1	802.0	1,070	941
3	HLX01	–1	802.0	1,208	1,085
4	HLX02	2,562	233.4	254	205
5	HLX03	–1	303.6	766	660
6	HLX03	–1	303.6	844	747
7	HLX04	2,557	466.8	1,132	1,043
8	HLX05	2,558	333.4	212	170
9	HLX06	2,559	666.7	355	284
10	HLX06	–1	668.3	403	321
11	HLX06	–1	668.3	450	358
12	HLX07	2,560	466.8	52	52
13	HLX07	–1	468.8	1,047	816
14	HLX07	–1	468.8	4,058	3,720
15	HLX08	2,561	2.4	644	533
16	KLX01	1,537	503.9	9,032	8,867
17	KLX01	1,528	618.1	10,000	10,000
18	KLX01	1,516	800.4		
19	KLX01	1,633	800.4		
20	KLX02	–1	1,333.4	775	605
21	KLX02	–1	1,333.9	832	650
22	KLX02	–1	1,336.3	821	642
23	KLX02	–1	1,340.4	768	601
24	KLX02	–1	1,346.4	745	583
25	KLX02	–1	1,354.2	680	534
26	KLX02	–1	1,363.8	625	491
27	KLX02	–1	1,375.1	589	464

Row no.	Idcode (borehole)	SNO	Dist to the sea m	Operational age model#1 = Baltic = 3,000; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS	Operational age model#2 = Baltic = 0; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS
28	KLX02	–1	1,388.1	583	460
29	KLX02	–1	1,402.8	537	423
30	KLX02	–1	1,419.0	548	432
31	KLX02	–1	1,436.7	525	414
32	KLX02	–1	1,456.0	525	414
33	KLX02	–1	1,476.6	504	397
34	KLX02	–1	1,498.6	518	408
35	KLX02	–1	1,521.9	533	420
36	KLX02	–1	1,546.5	528	416
37	KLX02	–1	1,572.2	593	467
38	KLX02	–1	1,599.0	822	643
39	KLX02	–1	1,627.0	4,876	4,638
40	KLX02	–1	1,655.9		
41	KLX02	–1	1,685.8		
42	KLX02	2,406	1,333.4	546	428
43	KLX02	2,413	1,337.6	538	422
44	KLX02	2,416	1,367.9	441	349
45	KLX02	2,421	1,393.5	473	373
46	KLX02	2,422	1,349.2	457	361
47	KLX02	2,424	1,425.6	445	352
48	KLX02	2,412	1,667.2	541	426
49	KLX02	2,418	1,609.5	543	429
50	KLX02	2,419	1,556.1	512	404
51	KLX02	2,420	1,463.7	475	375
52	KLX02	2,427	1,507.3	534	423
53	KLX02	2,705	1,370.8	1,163	931
54	KLX02	2,738	1,366.4	562	441
55	KLX02	2,712	1,543.9	3,170	2,956

Row no.	Idcode (borehole)	SNO	Dist to the sea m	Operational age model#1 = Baltic = 3,000; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS	Operational age model#2 = Baltic = 0; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS
56	PLX00013	2,523	2,933.4	440	348
57	PLX00014	2,524	2,733.4	453	357
58	PLX00015	2,526	1,466.7	241	191
59	PLX00017	2,528	1,133.4	530	449
60	PLX00018	2,529	1,666.7	1,053	1,008
61	PLX00020	2,531	3,300.0	395	315
62	PLX00021	2,532	434.0	539	424
63	PLX00022	2,533	541.6	1,964	1,780
64	PLX00023	3,031	373.0	394	312
65	PLX00023	2,534	373.0	228	181
66	PLX00024	2,535	296.9	284	226
67	PLX00025	2,536	251.0	183	146
68	PLX00026	2,537	236.0	272	216
69	PLX00027	2,538	209.4	256	204
70	PLX00030	2,541	0.0	2,677	505
71	PLX00031	3,016	0.0	3,000	0
72	PLX00031	2,542	0.0	2,826	566
73	PLX00032	2,543	75.3	437	347
74	PLX00033	2,544	66.8	1,313	1,302
75	PLX00034	2,545	800.0	50	39
76	PLX00035	2,546	500.0	47	37
77	PLX00036	2,547	102.1	31	24
78	PLX00037	2,548	68.0	0	0
79	PLX00038	2,549	0.0	123	95
80	PLX00039	2,550	0.0	3,094	772
81	PLX00040	3,017	0.0		
82	PLX00040	2,551	0.0		
83	PLX00041	2,552	2,166.7	475	376

Row no.	Idcode (borehole)	SNO	Dist to the sea m	Operational age model#1 = Baltic = 3,000; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS	Operational age model#2 = Baltic = 0; Surface = 0 Meteoric = 60; Deep Saline = 10,000 YEARS
84	PLX00042	2,553	2,067.0	2,755	2,431
85	PLX00043	2,554	0.0	566	446
86	PLX00044	3,010	59.6	566	78
87	PLX00045	3,011	46.8	840	0
88	PLX00046	3,012	34.0	270	0
89	PLX00047	3,013	17.0	3,283	2,241
90	PLX00048	3,014	25.5	2,818	1,801
91	PLX00049	3,015	38.3	1,925	907
92	PLX00050	3,018	129.4	178	142
93	PLX00051	3,019	121.8	349	275
94	PLX00052	3,020	118.0	475	374
95	PLX00053	3,021	106.7	802	626
96	PLX00054	3,022	159.9	846	659
97	PLX00055	3,023	236.0	296	237
98	PLX00056	3,024	228.4	312	249
99	PLX00057	3,025	220.8	390	309
100	PLX00058	3,026	190.3	464	365
101	PLX00059	3,027	15.2	1,644	1,268
102	PLX00060	3,028	7.6	1,888	1,105
103	PLX00061	3,029	1.6	697	546
104	PLX00062	3,030	274.1	490	387
105	PLX00063	3,032	7.7	465	369
106	PLX00064	3,033	2.2	861	671
107	PLX00065	3,034	61.0	1,104	855
108	Rain’60			60	60

–1.#ND indicates observations in the PCA outside the polygone and they are therefore not modelled.
Italics SO4 = Calculated from SO4-S
Bold Tr = Estimated values: elevation 0–800 m Tr = 22TU; elevation > 800 m Tr = 0TU
Underlined Mixing portion = Estimated values for samples close to the polygon
Greyshaded rows = Samples within the modelled area
Reference water

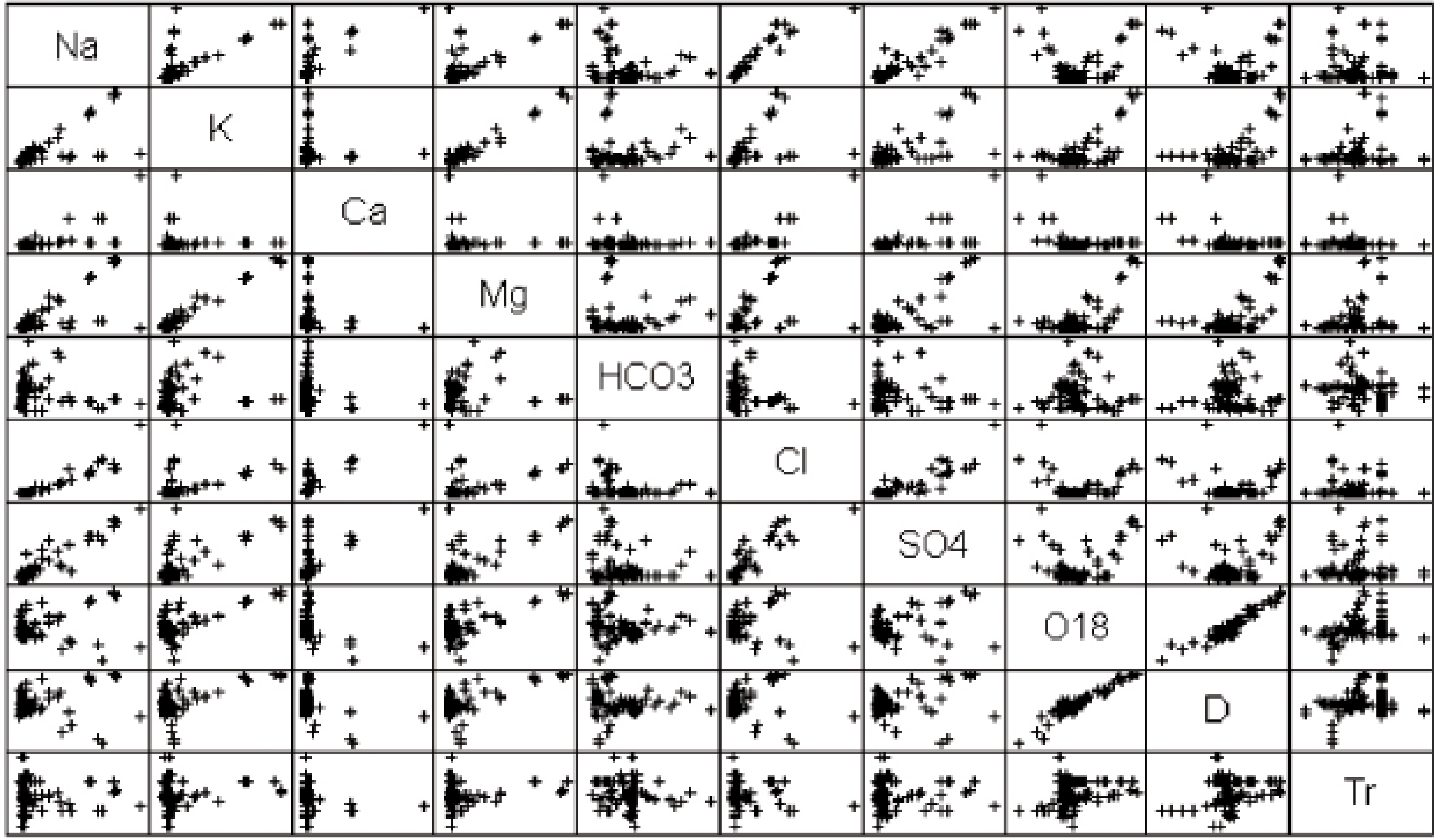


***Figure A1-2.** Multiplot of the major components, stable isotopes and tritium plotted as scatter plots.*

Appendix 2

Trace elements

Appendix 2 lists all the observations containing trace elements. The multi-plot (Figure A2-1) shows the degree of correlation between the analysed elements. The analytical data have been extracted from the SKB database SICADA. The major elements are given in mg/l, the stable isotopes in ‰, tritium in TU and the trace elements in µg/l.

Row	Idcode	SNO	Na	K	Ca	Mg	HCO3	Cl	SO4	O18	D	Tr	U	Th	Sc	Rb	Y
64	PLX00023	3,031	10.8	2.48	11.4	2.8	28	10.2	17.3	–9.9	–75.7	13.6	0.742	0.522	0.364	4.68	5.3
71	PLX00031	3,016	1,920	74.9	92.2	236	93	3,510	479.4	–6.1	–56.4	17.2	0.846	0.009	0.009	23.2	0.162
81	PLX00040	3,017	1,970	75.1	94.1	242	95	3,670	503.4	–6.5	–57.5	17.8	0.75	0.007	0.009	24.5	0.203
86	PLX00044	3,010	101	3.38	106	35	8	267	225.0	–7.6	–62.9	15.4	0.066	0.01	0.015	8.22	2.44
87	PLX00045	3,011	447	10.8	140	63.1	11	1,060	189.1	–7.3	–59.9	15.4	0.068	0.011	0.015	16.8	2.18
88	PLX00046	3,012	143	10.6	36	35.7	290	234	12.9	–7.9	–66.1	15.1	0.687	0.03	0.035	3.9	1.29
89	PLX00047	3,013	585	21	82.3	111	276	950	353.6	–9.3	–72.1	16	0.782	0.053	0.048	5.22	1.06
90	PLX00048	3,014	757	27.2	76.3	107	518	1,360	237.3	–9.1	–71.2	17.1	0.729	0.074	0.06	7.62	1.35
91	PLX00049	3,015	813	36	72.1	101	471	1,450	125.2	–8.6	–68.3	12.1	0.218	0.048	0.034	7.4	0.865
92	PLX00050	3,018	24.9	1.44	17	12	152	16.8	7.5	–9.2	–73	13.9	0.7	0.29	0.278	2.56	5.82
93	PLX00051	3,019	39.6	0.7	30	11.8	171	32	33.9	–9.4	–73.3	14.2	0.354	0.173	0.184	1.37	4.37
94	PLX00052	3,020	63.5	6.08	31.1	20.9	329	31.8	11.1	–10	–77.6	13.1	2.09	0.706	0.672	5.33	14
95	PLX00053	3,021	176	7.96	51.4	52	616	166	9.1	–10.3	–80.4	12.8	1.46	0.05	0.042	2.9	1.19
96	PLX00054	3,022	169	8.46	45.9	37.4	406	221	7.8	–10.1	–79	13.4	1.14	0.07	0.072	4.78	2.25
97	PLX00055	3,023	9.3	1.5	10.8	2.5	53	9.7	8.2	–9.7	–76.2	14.5	0.403	0.183	0.169	4.03	3.44
98	PLX00056	3,024	12.9	1.05	9.1	3.3	51	11.9	8.3	–9.9	–76	14.2	0.744	0.357	0.326	4.11	9.18
99	PLX00057	3,025	39.3	1.93	15.2	13.6	163	33.4	8.5	–9.9	–77.4	21.6	0.371	0.087	0.084	1.98	2.57
100	PLX00058	3,026	65.6	5.35	16.8	19	212	60.4	5.6	–9.8	–76.6	13.6	0.315	0.159	0.107	4.28	2.46
101	PLX00059	3,027	318	13.5	28.8	42.8	6	471	65.3	–9.4	–72	15.8	0.965	0.326	0.111	10.7	9.02

Row	Idcode	SNO	Na	K	Ca	Mg	HCO3	Cl	SO4	O18	D	Tr	U	Th	Sc	Rb	Y
102	PLX00060	3,028	565	20.6	47.1	77.2	93	900	163.6	–8.6	–68.6	14.2	0.277	0.114	0.041	9.89	2.56
103	PLX00061	3,029	139	2.04	24.4	20.6	156	244	5.0	–10.1	–77.4	15.3	0.166	0.064	0.048	1.29	1.47
104	PLX00062	3,030	44.8	2	18.1	16.3	179	39	14.4	–10.3	–77.9	16.4	0.409	0.112	0.079	2.28	2.1
105	PLX00063	3,032	33.3	3.21	16.2	6.2	103	33.6	1.8	–10.1	–80	14	0.311	0.163	0.146	3.54	3.82
106	PLX00064	3,033	137.5	6.88	21.3	27.2	177	219	25.2	–10	–76.3	14.8	0.379	0.005	0.069	2	1.62
107	PLX00065	3,034	269	15.4	29.8	38.5	426	376	16.6	–9.9	–75.2	10.5	1.05	0.073	0.08	5.9	1.47
a	KLX02	2,931	6,210	17.9	11,200	2.7	9	31,230	1,024.0	–9.7	–61.7	0.8	1.24	1.7292	0.574	138	1.28
b	KLX02	2,934	3,730	10.5	5,250	5	11	15,130	860.0	–11.4	–83.2	2.5	8.308	3.2619	0.0271	62.1	0.614
c	KLX02	3,035	1,280	9.4	1,680	20.5	63	4,730	377.0	–10.9	–79.1	8.4	56.792	3.0261	0.0942	35.2	0.313
d	KLX02	3,038	7,420	32.6	14,800	1.2	42	36,970	1,205.0	–9.3	–54.9	–	596.44	7.467	0.583	178	2.11

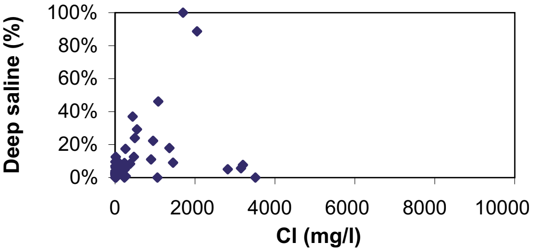
Row	In	Cs	Ba	La	Tl	Ce	Pr	Nd	Sm	Eu	Ho	Er	Tm	Yb	Lu
64	0.01	0.024	12.4	4.36	0.003	7.38	1.14	4.21	0.731	0.114	0.117	0.372	0.063	0.48	0.0926
71	0.005	0.055	22.8	0.063	0.007	0.103	0.0144	0.061	0.013	0.0032	0.0045	0.0125	0.002	0.013	0.0027
81	0.0072	0.054	19.3	0.037	0.009	0.058	0.0082	0.038	0.009	0.0036	0.0051	0.0151	0.003	0.015	0.0027
86	0.005	0.06	140	4.39	0.056	4.81	0.431	1.31	0.168	0.0315	0.0348	0.0989	0.014	0.092	0.0166
87	0.005	0.12	249	4.38	0.126	4.92	0.433	1.32	0.172	0.0322	0.0329	0.093	0.013	0.091	0.0172
88	0.005	0.01	48.4	1.22	0.003	2.28	0.288	1.08	0.179	0.0323	0.0296	0.0893	0.014	0.097	0.0187
89	0.005	0.008	79.8	0.531	0.001	0.981	0.134	0.55	0.109	0.0213	0.0271	0.0881	0.015	0.104	0.0205
90	0.005	0.01	68	0.764	0.001	1.42	0.193	0.78	0.157	0.0302	0.035	0.107	0.017	0.121	0.0239
91	0.005	0.009	108	0.323	0.001	0.611	0.0846	0.354	0.075	0.0168	0.0243	0.0795	0.014	0.098	0.0193
92	0.0431	7.91	31.9	4.24	0.004	7.91	1.08	4.09	0.719	0.118	0.123	0.368	0.057	0.391	0.071
93	0.0257	0.022	47.9	3.01	0.004	5.54	0.732	2.88	0.5	0.0855	0.0887	0.27	0.044	0.297	0.055
94	0.0158	0.082	61.7	12.1	0.004	21.9	2.9	10.6	1.85	0.303	0.315	0.931	0.147	1	0.176
95	0.0132	0.023	22.8	1.22	0.002	2.09	0.278	0.961	0.166	0.0266	0.0262	0.0737	0.011	0.076	0.0129
96	0.0079	0.044	73.2	2.18	0.002	3.9	0.492	1.8	0.312	0.0508	0.0472	0.137	0.022	0.141	0.0245
97	0.0186	0.046	14.2	4.26	0.004	8.44	1.04	3.7	0.605	0.0939	0.0779	0.224	0.034	0.232	0.0406
98	0.0255	0.073	18.8	9.34	0.002	19.1	2.59	9.53	1.6	0.242	0.18	0.518	0.08	0.547	0.0945
99	0.0188	0.018	8.42	3.04	0.001	5.59	0.707	2.49	0.399	0.0617	0.0514	0.149	0.022	0.144	0.024
100	0.0191	0.1	10.7	2.92	0.01	5.04	0.572	2.31	0.378	0.0588	0.0583	0.163	0.025	0.162	0.0272
101	0.005	0.146	57	8.42	0.01	16.6	2.29	9.11	1.72	0.236	0.251	0.752	0.118	0.914	0.157
102	0.0079	0.059	59.2	2.02	0.002	3.87	0.539	2.22	0.411	0.0525	0.0668	0.209	0.033	0.243	0.0505
103	0.0088	1.88	19.9	1.02	0.001	1.88	0.264	1.01	0.191	0.0282	0.0317	0.1	0.016	0.114	0.0208
104	0.0076	0.042	12.9	1.99	0.005	3.51	0.488	1.77	0.311	0.0482	0.0461	0.133	0.02	0.128	0.0212
105	0.0106	0.077	46.6	2.24	0.001	4.52	0.681	2.84	0.54	0.0778	0.0855	0.261	0.041	0.301	0.0559
106	0.0137	0.011	8.22	1.63	0.001	2.92	0.361	1.29	0.221	0.0359	0.0342	0.0995	0.015	0.105	0.0188
107	0.0081	0.0025	18.1	1.17	0.001	2.12	0.269	1	0.175	0.0295	0.0328	0.0981	0.016	0.111	0.0196
a	0.05	14.6	205	0.0239	0.005	0.0092	0.005	0.014	0.005	0.0065	0.005	0.005	0.005	0.0089	0.005
b	0.05	5.22	144	3.91	0.005	0.409	0.0184	0.066	0.005	0.005	0.005	0.0052	0.005	0.0052	0.005
c	0.062	2.88	291	0.334	0.465	0.136	0.02	0.0544	0.02	0.02	0.02	0.02	0.02	0.02	0.0200
d	0.119	18.6	424	2.27	0.577	0.594	0.05	0.163	0.05	0.05	0.05	0.05	0.05	0.05	0.0500

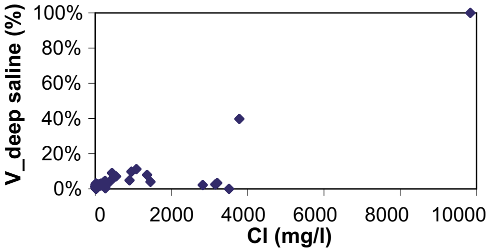
Figure A2-1. *Multiplot of the major components, stable isotopes, tritium and trace elements plotted as scatter plots.*

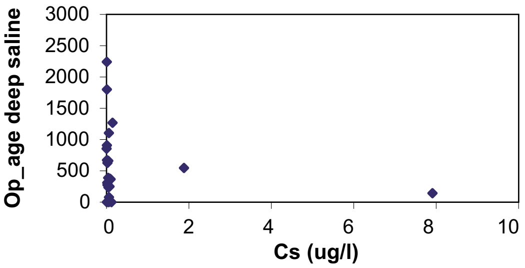
Appendix 3

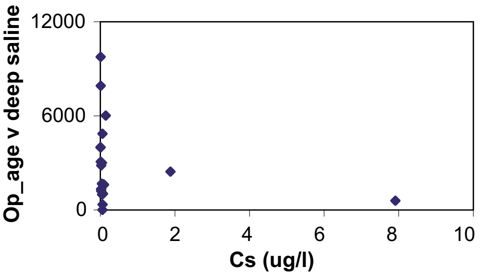
Correlation tests

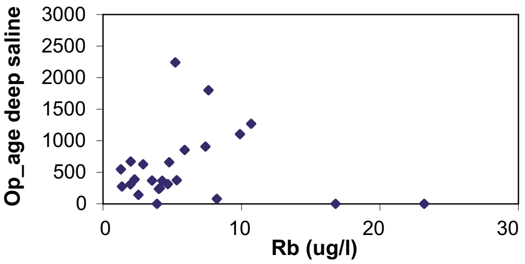
Appendix 3 shows different correlation tests performed on the data set used in this work. A correlation is obtained between some trace elements (Rb, Cs and to some degree with Th) and Cl (page 1). This correlation is only obtained when the Cl concentrations are high. At dilute waters and a depth of few meters there are no apparent correlations (page 3). The low element concentration can indicate strong dilution or that that the elements are affected by reactions or a combination of both. The total U and Th content sampled from the deep borehole KLX02 do not agree with the isotope analysis of these elements which may indicate analytical problems for these observations. The analytical data have been extracted from the SKB database SICADA and are listed in Appendix 1 and 2.

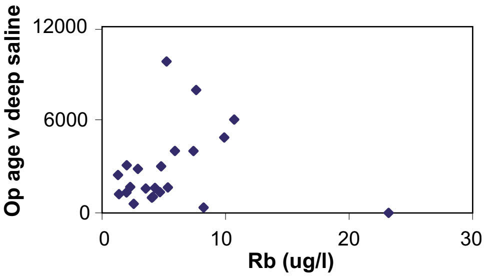

Deep saline (%)
100%
80%
60%
40%
20%
0%
0
2000
4000
6000
8000
10000
Cl (mg/l)

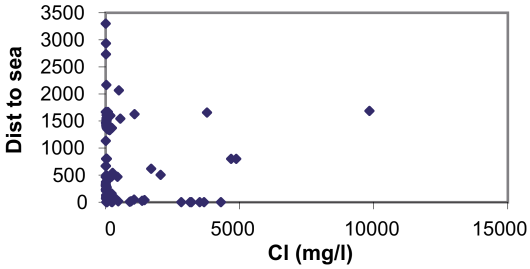

V_deep saline (%)
100%
80%
60%
40%
20%
0%
0
2000
4000
6000
8000
10000
Cl (mg/l)

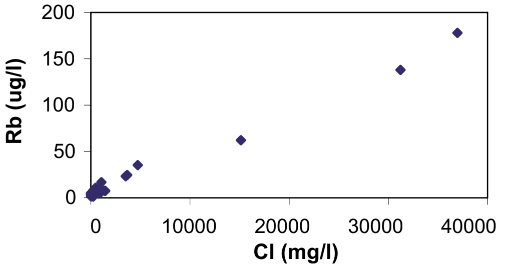

Op_age deep saline
3000
2500
2000
1500
1000
500
0
0
2
4
6
8
10
Cs (ug/l)

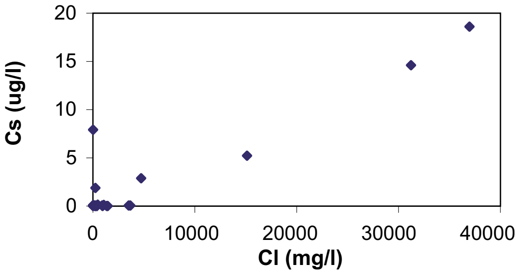

Op_age v deep saline
12000
6000
0
0
2
4
6
8
10
Cs (ug/l)

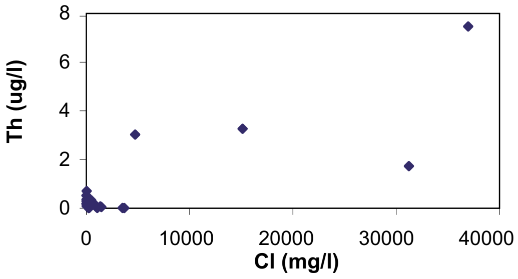

Op_age deep saline
3000
2500
2000
1500
1000
500
0
0
10
20
30
Rb (ug/l)

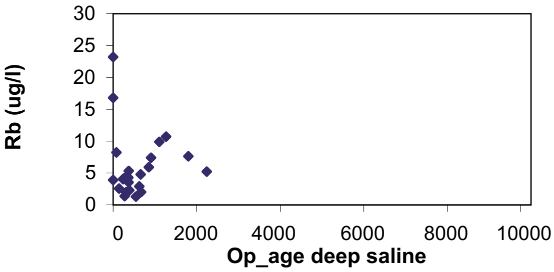

Op age v deep saline
12000
6000
0
0
10
20
30
Rb (ug/l)

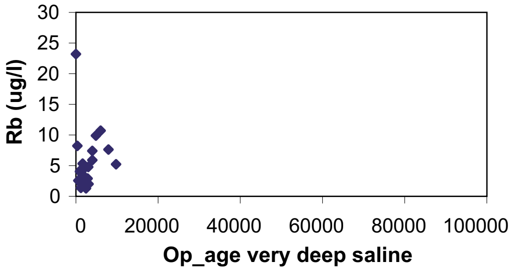

Dist to sea
3500
3000
2500
2000
1500
1000
500
0
0
5000
10000
15000
Cl (mg/l)

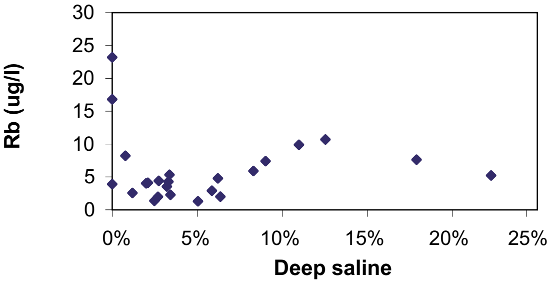

Rb (ug/l)
200
150
100
50
0
0
10000
20000
30000
40000
Cl (mg/l)

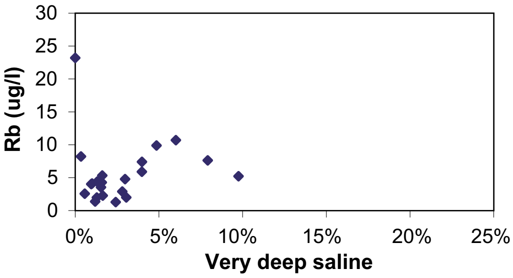

Cs (ug/l)
20
15
10
5
0
0
10000
20000
30000
40000
Cl (mg/l)

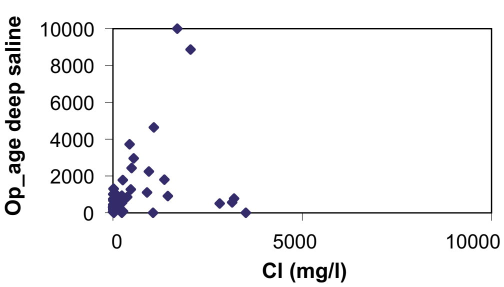

Th (ug/l)
8
6
4
2
0
0
10000
20000
30000
40000
Cl (mg/l)

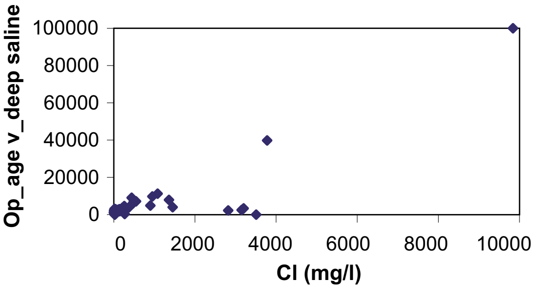

Rb (ug/l)
30
25
20
15
10
5
0
0
2000
4000
6000
8000
10000
Op_age deep saline

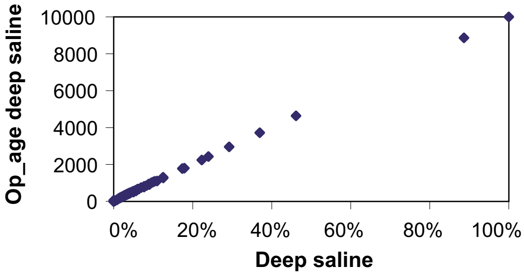

Rb (ug/l)
30
25
20
15
10
5
0
0
20000
40000
60000
80000
100000
Op_age very deep saline

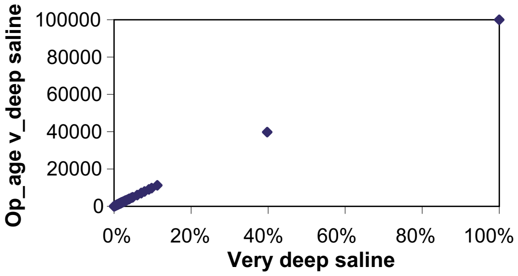

Rb (ug/l)
30
25
20
15
10
5
0
0%
5%
10%
15%
20%
25%
Deep saline

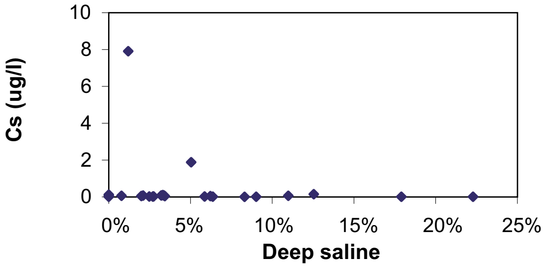

Rb (ug/l)
30
25
20
15
10
5
0
0%
5%
10%
15%
20%
25%
Very deep saline

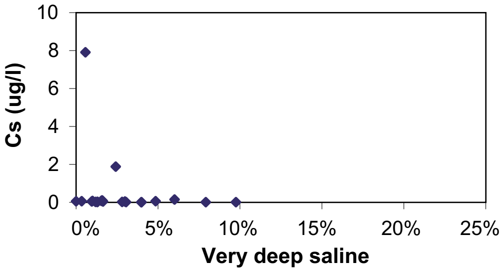

Op_age deep saline
10000
8000
6000
4000
2000
0
0
5000
10000
Cl (mg/l)

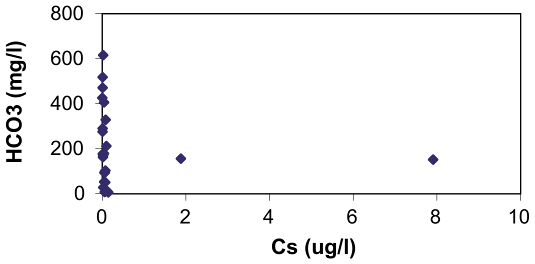

Op_age v_deep saline
100000
80000
60000
40000
20000
0
0
2000
4000
6000
8000
10000
Cl (mg/l)

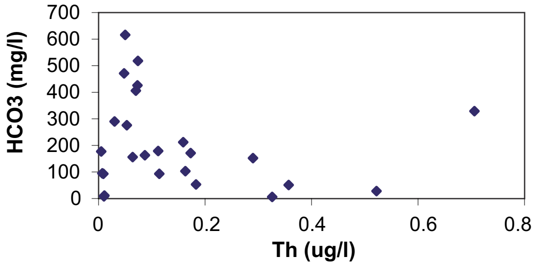

Op_age deep saline
10000
8000
6000
4000
2000
0
0%
20%
40%
60%
80%
100%
Deep saline

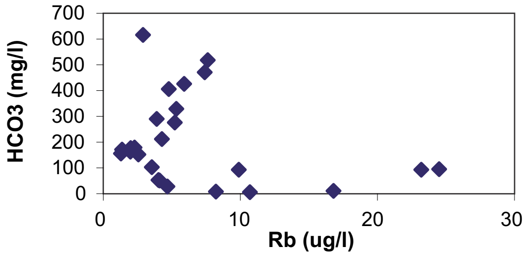

Op_age v_deep saline
100000
80000
60000
40000
20000
0
0%
20%
40%
60%
80%
100%
Very deep saline

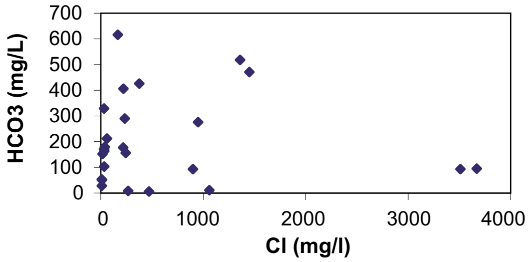

Cs (ug/l)
10
8
6
4
2
0
0%
5%
10%
15%
20%
25%
Deep saline

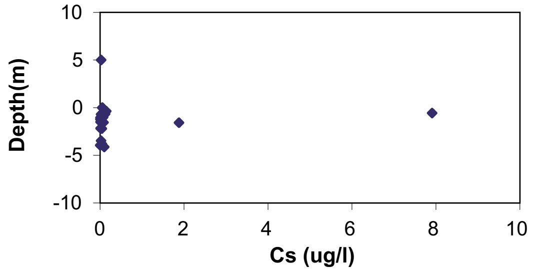

Cs (ug/l)
10
8
6
4
2
0
0%
5%
10%
15%
20%
25%
Very deep saline

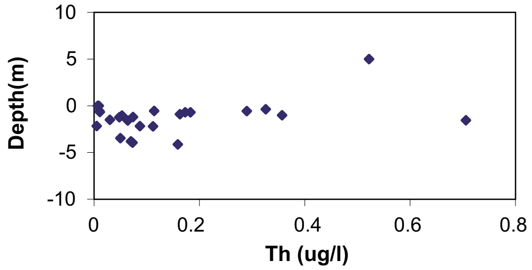

HCO3 (mg/l)
800
600
400
200
0
0
2
4
6
8
10
Cs (ug/l)

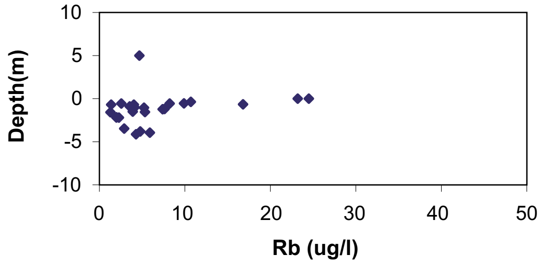

HCO3 (mg/l)
700
600
500
400
300
200
100
0
0
0.2
0.4
0.6
0.8
Th (ug/l)

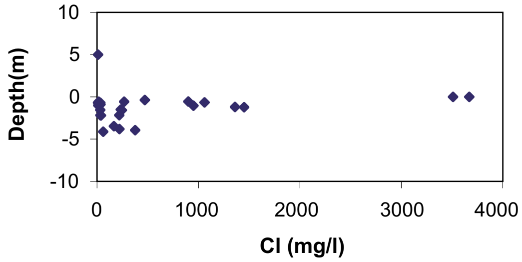

HCO3 (mg/l)
700
600
500
400
300
200
100
0
0
10
20
30
Rb (ug/l)

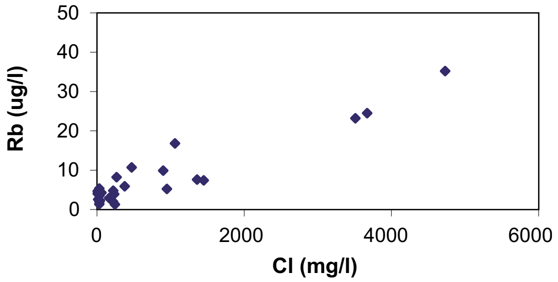

HCO3 (mg/L)
700
600
500
400
300
200
100
0
0
1000
2000
3000
4000
Cl (mg/l)


Depth(m)
10
5
0
-5
-10
0
2
4
6
8
10
Cs (ug/l)


Depth(m)
10
5
0
-5
-10
0
0.2
0.4
0.6
0.8
Th (ug/l)


Depth(m)
10
5
0
-5
-10
0
10
20
30
40
50
Rb (ug/l)


Depth(m)
10
5
0
-5
-10
0
1000
2000
3000
4000
Cl (mg/l)


Rb (ug/l)
50
40
30
20
10
0
0
2000
4000
6000
Cl (mg/l)

Appendix 4

Alternative M3 calculation including very deep brines

This appendix (Figure A4-1) shows an alternative M3 calculation when the deep saline end member (KLX0: –440 m no. 17 in Appendix 1) was replaced by the very deep saline end member (no. 41 in Appendix 1) compare with Figure 5-3. The M3 results from this modelling were used for the visualisation of the "very deep box" in Appendix 6 (Section 15.2).

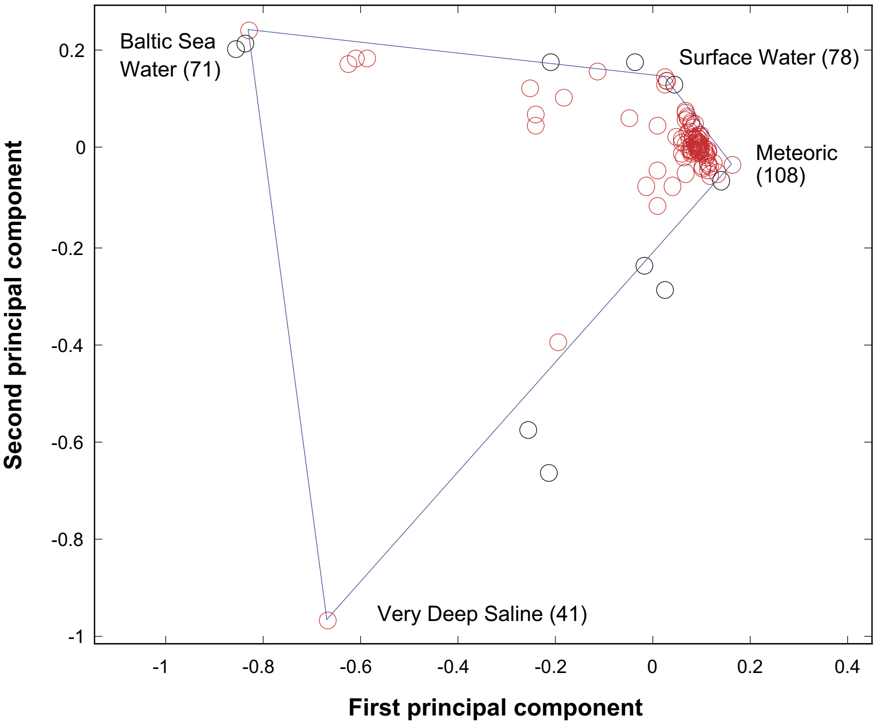


***Figure A4-1.** PCA of Laxemar samples showing the Very Deep Saline reference water (KLX02: –1,031.5 m). The first and second principal components summarise 73% of the total information in the variables.*

Alternative M3 calculation including distance to the sea

Appendix 5 (Figure A5-1) shows a test where the distance from the sampling point to the sea was included in the PCA. This was done to illustrate how the PCA is affected by including additional information.

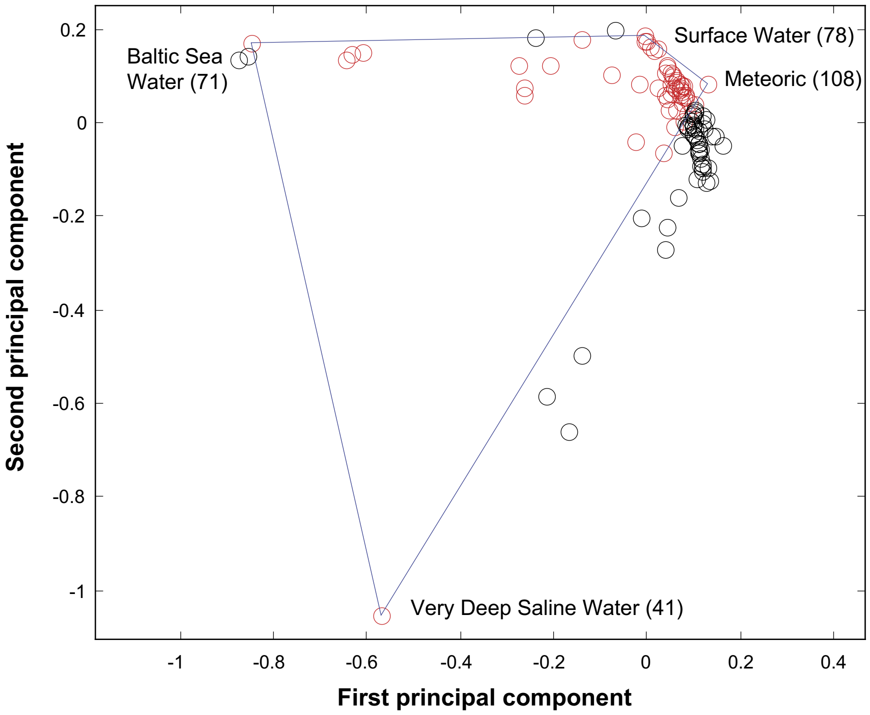


Figure A5-1. *PCA of Laxemar samples including the variables depth (elevation) and the calculated distance from the Baltic Sea and by using the following reference waters: meteoric, Baltic Sea, surface and very deep saline. There are similarities between the figure A4-1 presented at Appendix 4 and this picture, despite a shift of the meteoric reference water. The first and second principal components summarise 66% of the total information in the variables which indicate a slightly more complex data set than for the one used in Figure A4-1 in Appendix 4.*

Appendix 6

Spacial scale effects

The visualisation of the extended profile towards NW (Enlarged box) and the extended box towards the depth of 1,000 m (Very deep box) are presented in this appendix. The general conclusion from extending the modelled area is that despite changing the scale the overall interpretations of the modelling remains unchanged compared with the visualisations in Sections 6.1 and 6.2.

A6.1 Enlarged box

For comparison the modelled area presented in Section 6.2 was extended towards NW (see black box in the Figure 3-1) in order to include more groundwater samples with possible evidence of influences from deep saline water. In the following modelling the transect NW-SE is analysed. The transect was orientated along the discharge area, where there are also the sampling points containing a calculated portion of deep saline water more than 10% (see Figure 5-4). The following features of the profiles were visualised:

- Calculated mixing proportions with M3 of Meteoric, Shallow, Baltic and Deep saline waters (the same deep saline water as used in the model "superficial box").
- Measured values of: Cl and oxygen-18.
- Calculated values of the operational age based on the reference water ages.
- Measured and calculated M3 deviation of the elements Ca, HCO_3 and SO_4 (positive value = gain, negative value = loss of element accounted by reactions).

The M3 modelling is based solely on chemical information, which can be used to support the 3D understanding of groundwater flow through the site area. The calculated mixing proportions are always relative to the selected reference waters. The results of the Voxel interpolations are shown in Figures (A6-1 to A6-7). The numerical results of the M3 mixing and deviation calculations for all observations are listed in Appendix 1.

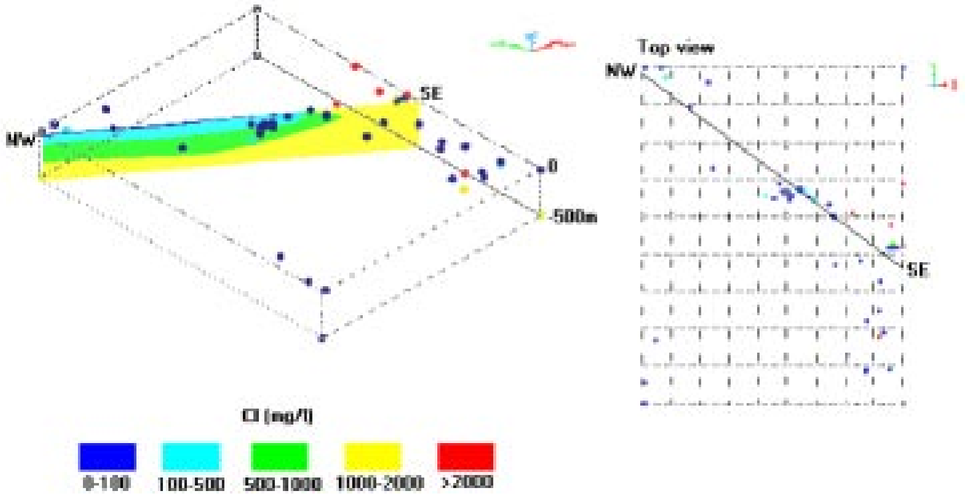


Figure A6-1. Visualisation of the sampling points, interpolation grid and location of the transect NW-SE (for orientation see Figure 3-1). A perspective view and a top view are presented. The concentration of Cl is shown in the sampling points, as well as along the cutting plane.

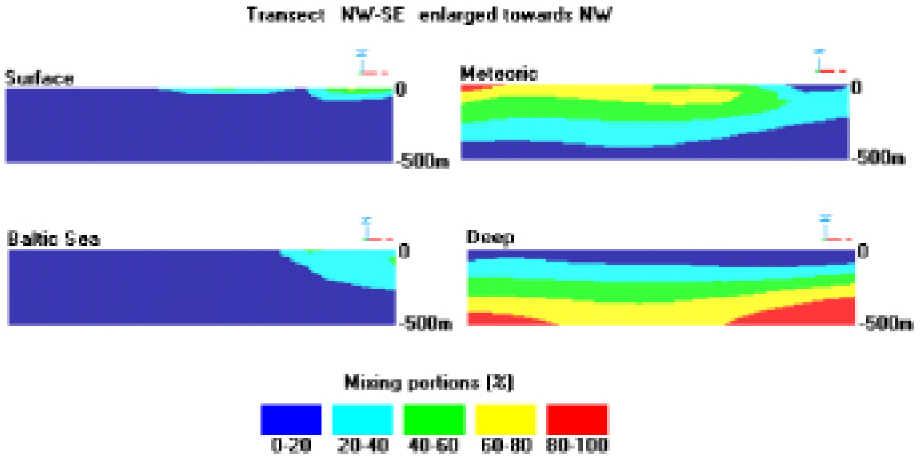


Figure A6-2. *Result of interpolation of calculated mixing proportions based on M3 calculations for Meteoric, Baltic Sea, Surface and deep saline water along the transect NW-SE (for orientation see Figure 3-1).*

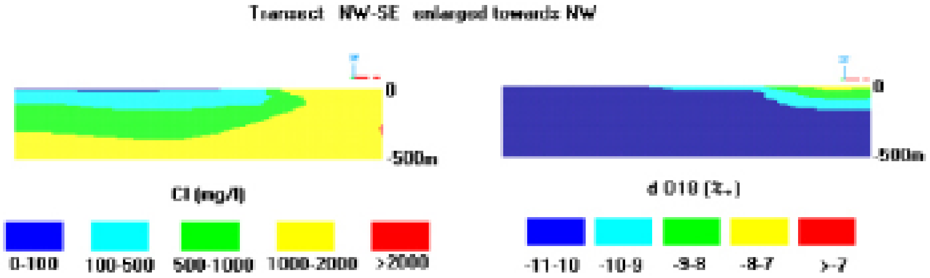


Figure A6-3. *Result of the Cl and O^{18} interpolation of measured values along the transect NW-SE (for orientation see Figure 3-1). The Cl profile indicates a possible interaction of salinity contribution from deeper water (lower right part of the profile) and the upper right part of the profile represents influences of Baltic Sea water. The $\delta^{18}O$ profile indicates a higher value for water associated with Baltic Sea water and a lower value for surface and shallow water. The lower the value the longer the possible residence time of the water is believed to be. The mean value of $\delta^{18}O$ of the annual precipitation is –10.*

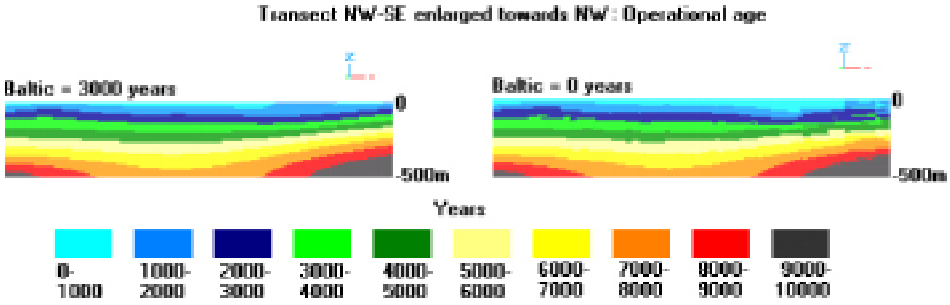


Figure A6-4. *Result of the calculated operational age along the transect NW-SE (for orientation see Figure 3-1) based on the reference waters ages: Meteoric water = 40 years, Surface water= 0 years, Deep saline water = 10,000 years. For the Baltic Sea water two cases are considered: Baltic Sea = 3,000 years (the left model) and Baltic Sea = 0 years (right profile). Both models show an increase of the operational age with depth. The operational age has the same distribution as the deep saline water in Figure A6-2 but different from Cl distribution in Figure A6-3.*

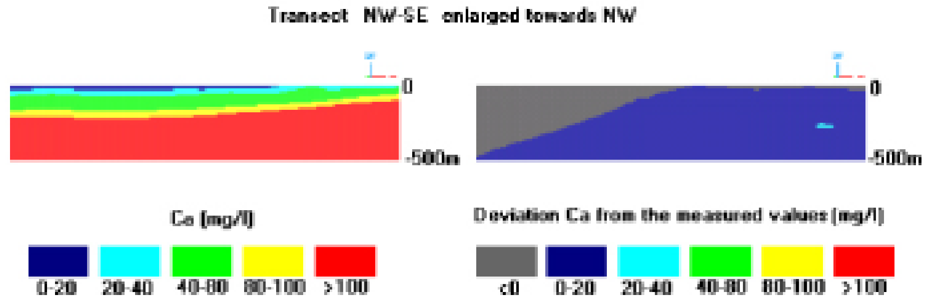


Figure A6-5. *Result of the Ca interpolation of measured values along the transect NW-SE (for orientation see Figure 3-1). Theleft figure shows that a possible source for Ca is Sea Water (upper right part of the profiles) and also from possible reactions such as calcite dissolution. The right figure shows the result of the Ca deviation not accounted for by transport in M3. A positive value indicates a gain a negative value a loss possible due to reactions. The profile indicates a loss of Ca at the surface. A gain is indicated in the middle and lower part of the profile.*

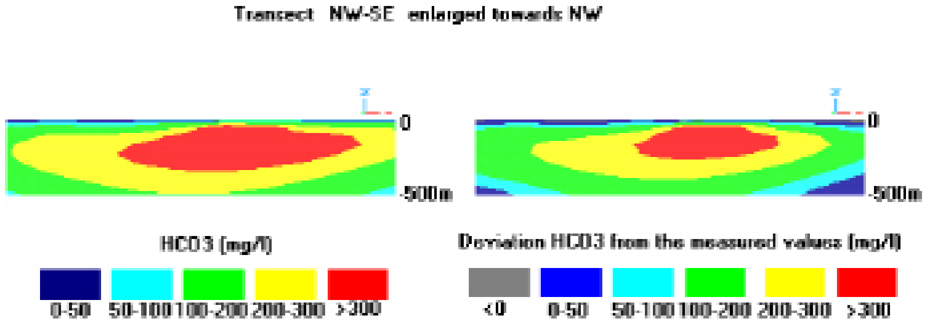


Figure A6-6. *Result of the HCO_3 interpolation of measured values along the transect NW-SE (for orientation see Figure 3-1). The model indicates a complex source for the measured HCO_3 content. The right figure shows the result of the HCO_3 deviation not accounted for by transport in M3. A positive value indicates gain a negative value a loss possible due to reactions. The model indicates a complex gain of HCO_3 possible from biogenic activity or calcite dissolution. Sulphate reduction associated with the Marine sediments can cause a gain of dissolved HCO_3 in the groundwater.*

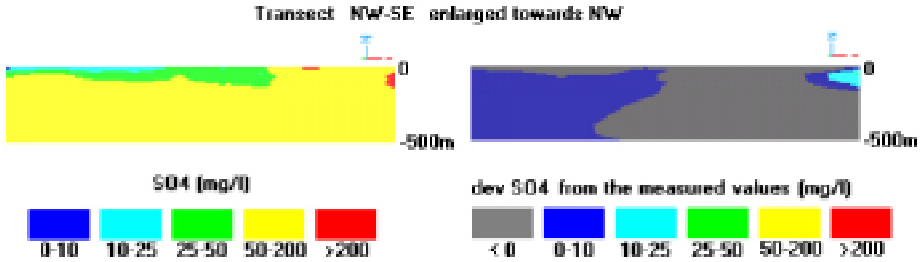


Figure A6-7. *Result of the SO_4 interpolation of measured values along the NW-SE (for orientation see Figure 3-1). The profile indicates a complex source for the measured SO_4 both from Sea and Deep water. The right figure shows the SO_4 deviation not accounted for by transport in M3. A positive value indicate a gain a negative value a loss possible due to reactions. The profile indicates a gain of SO_4 below the Sea and from the Deep water. A loss is indicated in the middle and upper part of the profiles. Areas with loss of SO_4 in combination with gain of HCO_3 (cf. Figure A6-6) can indicate areas with sulphate reduction associated with the marine sediments.*

The M3 modelling indicates that the surface and shallow groundwater system is complex. The upper groundwater system includes interaction between different water types and reactions such as inorganic and biogenic reactions. The deep box model brings more indication about the interaction from the deep saline water type. Chloride, used in classical modelling as a good conservative tracer, cannot be used to explain this complex system. This is put in evidence by the fact that the operational age is not correlated with Cl. The operational age is correlated with the deep saline water type in particular, but not the Cl content that has several sources.

A6.2 Very deep box

For comparison the modelled area presented in Section 15.1 was extended to the depth of 1,000 m in order to include in the model the very deep saline water (no. 41 in Appendix 1 instead of no.17 as used in modelling above). The results of the PCA are shown in Appendix 4 (Figure A4-1). In the modelling the transect NW-SE was studied. As presented in Figure 5-4, the transect was orientated along the discharge area, where the sampling points contained a calculated portion of deep saline water more than 10%. The aim is to model and visualise the influence of deep saline water type on the biosphere. The following features of the profiles were visualised:

- Calculated mixing proportions with M3 of Very Deep saline waters.
- Measured values of Cl.
- Calculated values of the operational age based on the reference waters ages.

The M3 modelling is based solely on chemical information which can be used to support the 3D understanding of groundwater flow through the site. The calculated mixing proportions are always relative to the selected reference waters. The results of the Voxel interpolations are shown in Figures (A6-8 to A6-10).

The M3 modelling indicates that in deeper systems (very deep saline water and at very large depths = 1,000 m) the Cl distribution is similar in the deeper part of the model with the very deep saline water distribution. The operational age correlate with the deep saline mixing portion calculation.

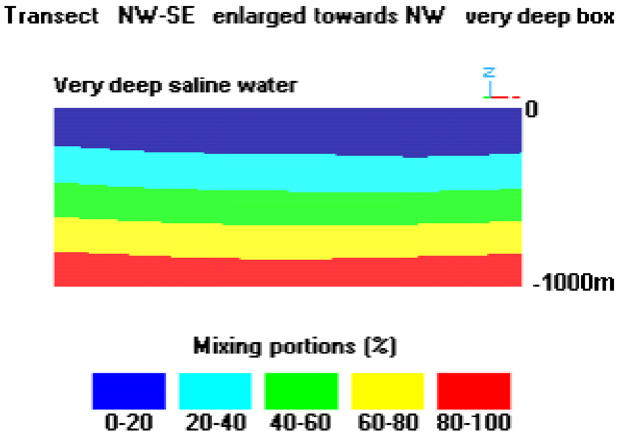


Figure A6-8. *Result of interpolation of calculated mixing proportions based on M3 calculations for Very deep saline water along the transect NW-SE (for orientation see Figure 3-1).*

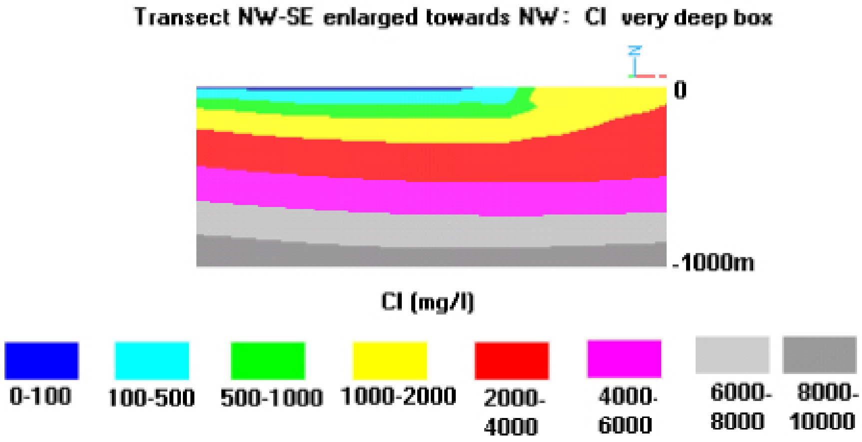


***Figure A6-9.** Result of the Cl interpolation of measured values along the transect NW-SE (for orientation see Figure 3-1). The Cl profile indicates a possible interaction of salinity contribution from deeper water and/or influences of the Baltic Sea water at the upper right part of the profile.*

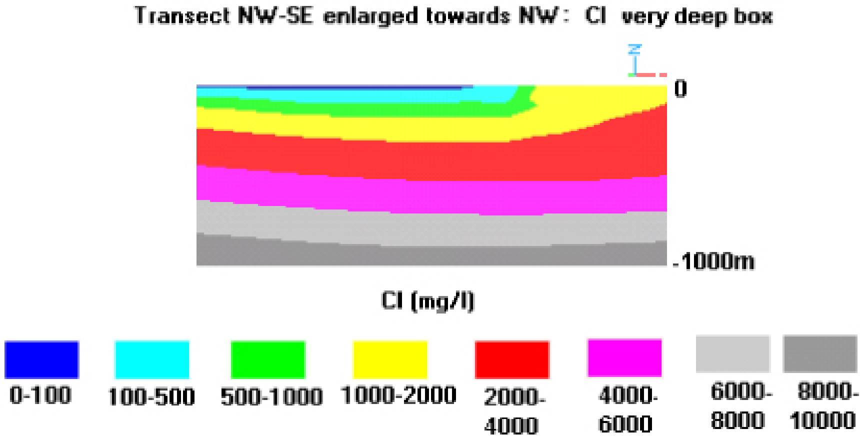


***Figure A6-10.** Result of the calculated operational age along the transect NW-SE (for orientation see Figure 3-1) based on the reference waters ages: Meteoric water = 40 years, Surface water = 0 years, Very Deep saline water = 100,000 years, Baltic Sea = 0 years. The model shows an increase of the operational age with depth. The operational age has the same distribution as the very deep saline water.*