Technical Report

TR-01-37

Demonstration of M3 modelling of the Canadian whiteshell research area (WRA) hydrogeochemical data

OPG / SKB M3 modelling project

M Laaksoharju, C Andersson, I Gurban
DE&S/Intera KB, Ottawa/Stockholm

M Gascoyne
Gascoyne GeoProjects Inc., Pinawa

April 2000

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

Demonstration of M3 modelling of the Canadian whiteshell research area (WRA) hydrogeochemical data

OPG/SKB M3 modelling project

M Laaksoharju, C Andersson, I Gurban
DE&S/Intera KB, Ottawa/Stockholm

M Gascoyne
Gascoyne GeoProjects Inc., Pinawa

April 2000

Keywords: WRA data, Canadian groundwater, URL, groundwater modelling, mathematical modelling, mixing calculations, mass-balance calculations, M3

ABSTRACT

This report describes the application of a new groundwater chemical modelling tool, the Multivariate Mixing and Mass balance modelling technique (M3) to Canadian Whiteshell Research Area (WRA) hydrogeochemical data. In particular, data from the site of the Underground Research Laboratory (URL) has been modelled, in order to test the potential of M3 as a modelling tool in the site description and evaluation process for nuclear fuel waste disposal. In M3 modelling the assumption is that the groundwater chemistry is a result of mixing as well as water/rock reactions. The M3 model uses the measured hydrogeochemical data for a site, determines the similarities and differences of groundwater compositions using a standard statistical method, and then quantifies the contributions of end-member components of groundwater mixing and additional water-rock interactions that modify groundwater composition.

The modelled present-day groundwaters at the URL site consist of a mixture in varying amounts of the following water types: meteoric precipitation, glacial, saline, brine and a type we classify as 'biogenic'. The results of the M3 mixing calculations indicate that the upper part of the bedrock (0-100m) is dominated by precipitation type water (100-40%). At greater depths (100-400 m) the precipitation water is replaced by biogenic water (40-100%). At depths 300-600m and in the NNW part of the URL area, glacial water (40-80%) that probably recharged during the last deglaciation dominates. In the NNW and SSE parts and at the same depth interval as the glacial water (300-600m) the influences from saline (5-20%) and brine (5-20%) type of water are detected. The draw-down from the URL shaft increases the portions of meteoric precipitation and biogenic water but may have flushed out historical waters such as glacial, saline and brine from the near vicinity of the shaft. The M3 mass-balance modelling indicates that there is a gain of HCO_3 not accounted for by mixing that is believed to be due to organic decomposition in the biogenic water type. At greater depths and in the NNW part of the bedrock the modelling indicates a loss of HCO_3 which could be due to calcite precipitation. The occurrence and the distribution of water types and the mass-balance calculations for carbonate are in general agreement with previous interpretations of groundwater composition and modelling of the site.

LIST OF CONTENTS

1 INTRODUCTION TO THE TASK

Characterisation of a site for nuclear fuel waste disposal typically involves taking thousands of measurements and developing site-specific models in each of several scientific and engineering disciplines. These models are usually independent of each other, and are sometimes inconsistent. Combining such models into a defensible, self-consistent understanding of the site characteristics has been problematic, and presenting this understanding in a clear and concise manner to stakeholders has proven to be difficult. This is an area where there is rather limited experience and therefore Ontario Power Generation (OPG) in Canada and the Swedish Nuclear Fuel and Waste Management Company (SKB) approved a test of a new groundwater modelling technique to see if the results can be used to address this issue. The data set used for the test was a Canadian database describing the hydrochemistry at the Whiteshell Research Area (WRA) in southeastern Manitoba and, in particular, at the Underground Research Laboratory (URL) site. The URL site contains a number of deep bedrock boreholes from which many groundwater samples have been taken and analysed to build up a comprehensive data set (Gascoyne, 2000).

The evolution of the groundwater composition is strongly related to the present and past flow conditions. As this is a continuous process, the type of infiltrating water as well as the existing water in the rock constantly change their compositions. The solute and isotopic content of groundwater samples can be interpreted as either the result of geochemical reactions between the groundwater and the minerals it contacts, or as the mixing of groundwater types of different origins or end-members (and hence different chemical signatures), or as a combination of both processes. Software tools to address these topics are under development in the international waste management community. One such tool is the Multivariate Mixing and Mass balance (M3) model developed by SKB (Laaksoharju et al., 1999a). M3 has been used at the Äspö Hard Rock Laboratory in Sweden (Laaksoharju, 1999b), the natural analogue Oklo in Gabon (Gurban et al., 1998), and the uranium ore deposit at Palmottu in Finland (Laaksoharju, 1999c). M3 is an interpretative technique that performs a cluster analysis (using multivariate principal component analysis) to identify waters of different origins, infer the mixing ratio of these end-members to reproduce each sample's chemistry, identify any deviations between the chemical measurements of each sample and the theoretical chemistry from the mixing calculation, interpret these deviations as resulting from interactions with the solid minerals, and interpret the spatial distribution of these reactions. As mixing of different groundwater types from various identified sources (i.e. end-members) can also be handled by hydrodynamic models, this provides an excellent opportunity to mathematically interface hydrochemistry with hydrogeology. The aim of the project is to demonstrate the potential for the M3 method rather than to perform a detail modelling of the WRA data set.

2 SITE DESCRIPTION AND CHARACTERISATION STUDIES

The concept for disposal of Canada's nuclear fuel waste is disposal of used fuel packaged in corrosion-resistant containers emplaced in an excavated vault at a nominal depth of 500-1000 m in a crystalline rock formation of the Canadian Shield (AECL 1994). Several studies have been conducted in order to understand and characterise the long term effects of the influences on the groundwater geochemical environment of the vault, e.g. Gascoyne (1996,1997), Gascoyne et al. (1991,1997), Kotzer et al. (1998). Because the principal mechanism for transport of radionuclides from the waste disposal vault to the biosphere is expected to be via groundwater advection and diffusion within pores and fractures in the rock, considerable attention has been given to both the hydrogeological and hydrogeochemical propoerties of groundwater in the rock.

The URL was constructed by Atomic Energy of Canada Limited (AECL) in a previously undisturbed portion of the granitic Lac du Bonnet batholith near Lac du Bonnet, Manitoba, Canada. A number of experiments have been conducted in the URL and the surrounding area of the WRA to assess aspects of the disposal concept. The compositions of groundwaters sampled at the URL represent the principal part of the WRA dataset used in this report.

Figure 1 shows a section through the URL lease area. The figure illustrates the complete flow system, from the groundwater recharge areas in the southeast and on the URL facility outcrop, through vertical fractures and deep, low-dipping fracture zones, to the discharge area in the northwest; included are groundwater compositions and salinities (as total dissolved solids, TDS).

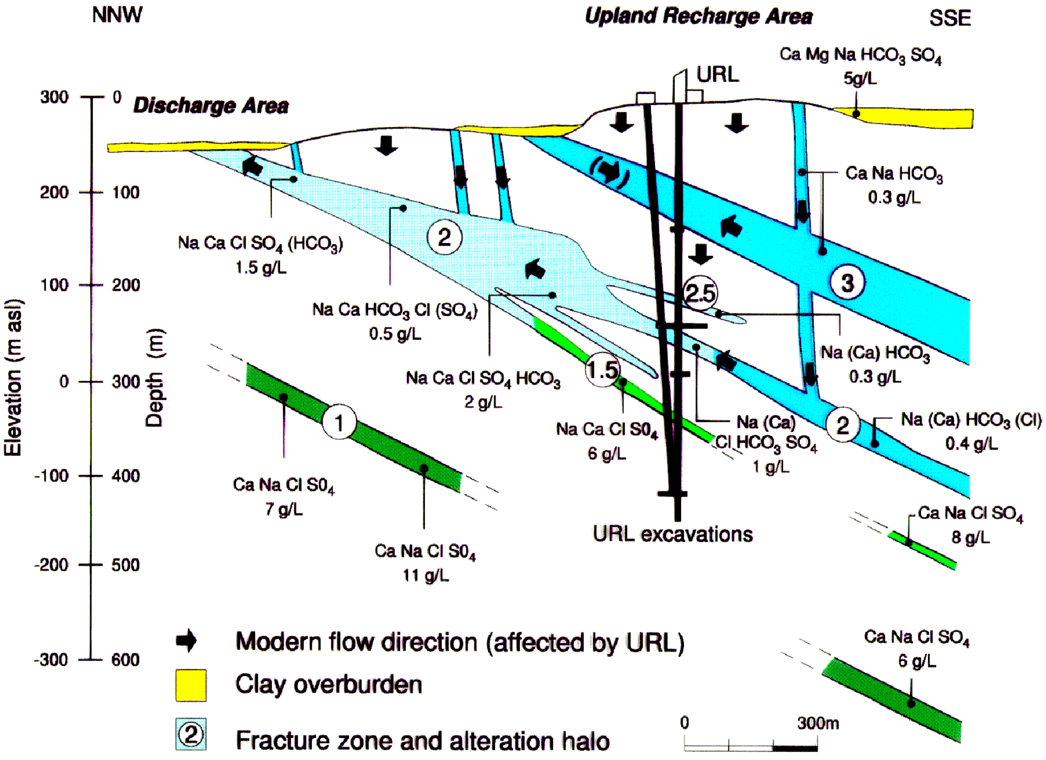


Figure 1: *Hydrogeologic section through the URL area. Groundwater compositions and salinities (TDS) are based on pumping and sampling numerous boreholes in the WRA. The flow directions are based on pre- and post-excavation head distributions (Gascoyne, 1997).*

The hydrogeologic section in Figure 1 shows that the near-surface groundwater in Fracture Zone 3 (FZ3) and near-vertical fractures is typically Ca-HCO_3 in composition. The groundwater evolves to a Na-HCO_3 composition in the deep recharging portion of the underlying FZ2 and, as it flows up the dip of the fault toward the surface, dissolved salt content increases and the water becomes brackish. At greater depths in the URL area, and elsewhere in the batholith, brackish and saline (Ca-Na-Cl or Na-Ca-Cl) groundwater predominates. This groundwater commonly has isotopic (δ^2H - $\delta^{18}O$) characteristics that indicate recharge under cold-climate conditions (at least 8,000 years ago) or, in the case of deeper, highly saline groundwater, under warm-climate conditions that are interpreted as being pre-glacial, i.e., $>10^6$ yr old (Gascoyne 1997; Gascoyne and Chan, 1992; Gascoyne, 1994). In some locations, this groundwater exists in isolated fracture zones of limited extent that are poorly connected to the near-surface fracture network. However, in other locations, saline groundwater occurs at depths of <100 m in highly permeable fractures and is moving toward discharge locations at the surface. An example of this phenomenon is shown on the left of Figure 1, where groundwater in FZ2 has a salinity of 1.5 g/L but is only 40 m below the surface. Hydraulic-head information shows that artesian conditions exist in FZ2 at this location, indicating that groundwater discharge is occurring at the base of the overburden above the subcrop of FZ2 (Gascoyne, 1997).

3 DATA COMPILATION AND EVALUATION FOR FURTHER M3 MODELLING

The data set used in this work was compiled based on the published WRA data. The following additional information was added to the data (see Appendix 1):

- Data for meteoric precipitation
- An estimate of the isotopic composition of glacial melt-water

Based on literature studies, scatter plots of the data, and the spatial distribution of the samples, the WRA data is believed to be appropriate for M3 modelling because:

- The analytical data comprise major components and isotopes (which together can reveal the information concerning the flow and reactions affecting the groundwater)
- The water samples represent different depths
- The hydrogeological model supports the inference that mixing of different water types may occur.
- The water samples appear to be derived from different water types

In addition a test was conducted on WRA data, where the possible influence of several end-members on the groundwater and the potential for ambiguity were determined by using a simple correlation test between water conservative constituents Cl and $\delta^{18}O$ (Figure 2). If the correlation is low (as in this case) there are two or more end-members involved in the groundwater system and a multivariate approach such as M3 can be employed.

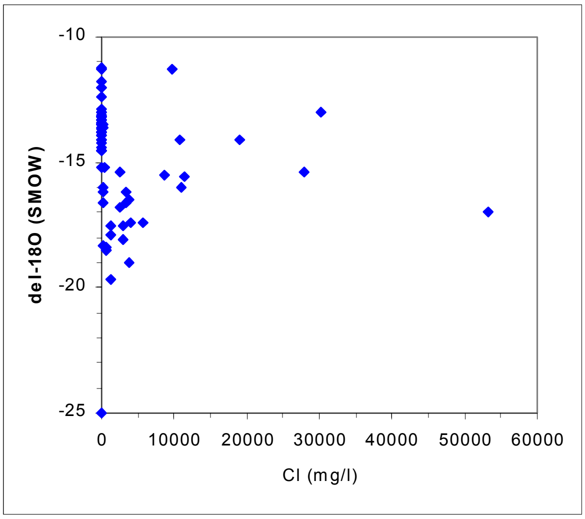


Figure 2: *Scatter plot of Cl versus $\delta^{18}O$ used to show that these water conservative elements indicate low correlation implying a complex origin for WRA's groundwaters.*

4 DESCRIPTION OF M3 MODELLING

Traditionally groundwater modelling consists of comparing the properties of different samples from which conclusions are drawn concerning the evolution of the groundwater at a site. M3 makes this comparison work by means of a mathematical model. The result of the modelling is presented as the contribution of mixing (%) and geochemical reactions (mg/l) to the measured groundwater composition. The modelling is based on the following assumptions: 1) groundwaters of similar compositions have undergone similar mixing and reactive processes, 2) groundwater composition is a good tracer for the flow and geochemical evolution of the groundwater and 3) the resulting groundwater is a mixture of different water types. The uncertainties in these assumptions are handled in the modelling by giving uncertainty ranges to the reported values.

The M3 model consists of three steps: the first step is a standard principal component analysis, the second is mixing, and the third is mass balance calculations. As an example, Figure 3 shows the modelling steps applied to the Äspö Hard Rock Laboratory data. An identical procedure as described in detail below, was followed in the WRA case study.

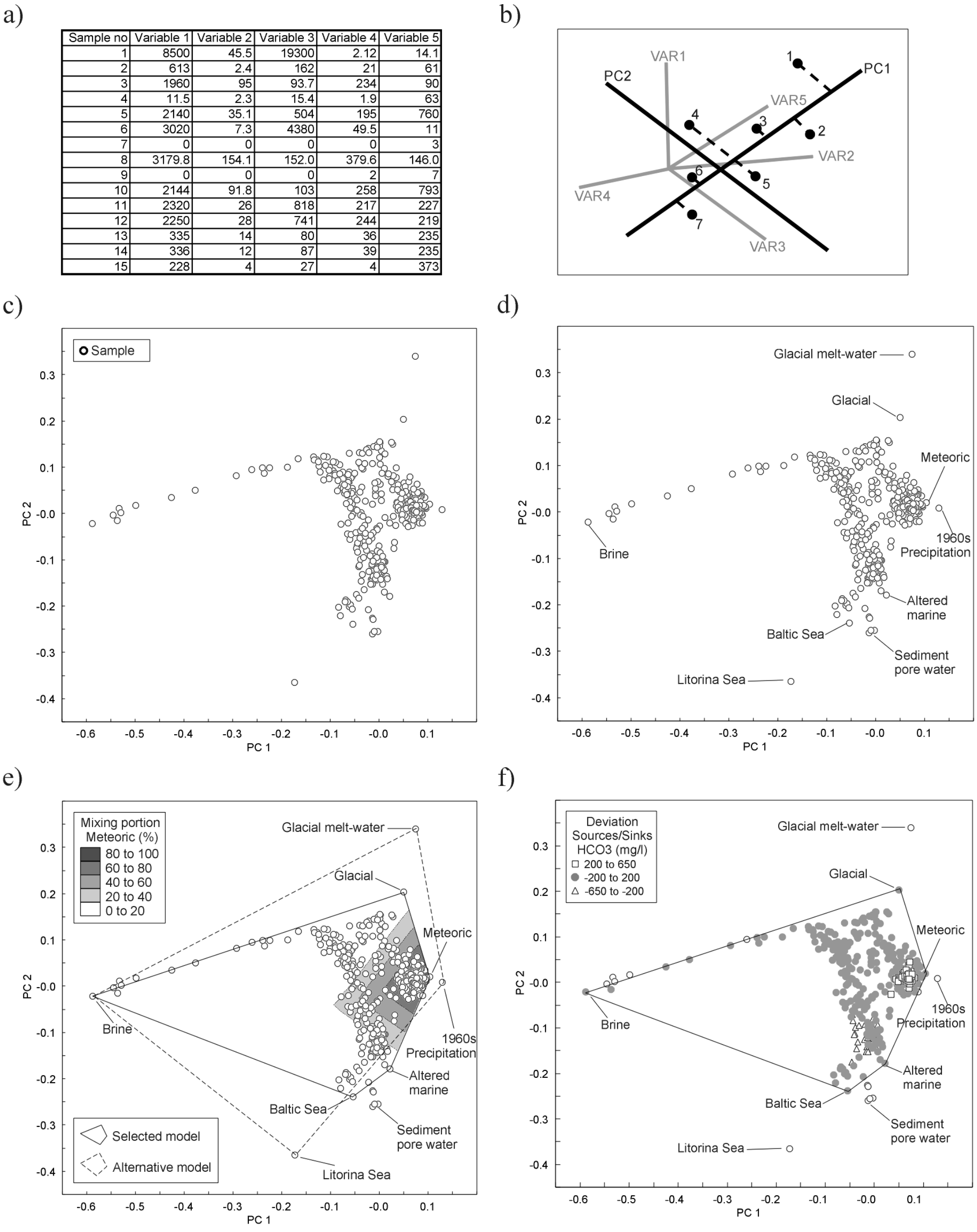
1) A *Multivariate* technique called Principal Component Analysis (PCA) is used for the clustering of the data to summarise the information and to construct an *ideal mixing model* for the site. Generally, the major components Cl, Ca, Na, Mg, K, SO_4 and HCO_3, in combination with the isotopes δ^2H, δ^{18}O and ^{3}H are used. If there is a lack of isotope data the modelling can still be performed but generally with a lower resolution as isotope compositions may contain useful information concerning the flow system. PCA aims to describe as much of the information from the ten variables in the first principal component as possible by using relative weighting of correlation coefficients. As much as possible of the remaining information is described by the second principal component. The principal components are equations of linear combinations that describe most of the information in the data. The weights for the different variables in the equations are calculated automatically by the PCA. For the Äspö data set, the first two principal components describe 70% of the information in the data set. The third or fourth principal components generally do not contain useful information but this depends on the complexity of the examined data and the chosen variables. If the first two principal components contain most of the information, an x, y scatter plot can be drawn. The x is the equation for the first principal component and y the equation for the second principal component. The plot is named the M3 plot and is used to visualise the clustering of the data as well as to identify reference waters. A reference water is a selected water composition used to compare with other samples. A reference groundwater can be any water composition included in the PCA but generally end-member compositions (extreme waters which may contribute to the groundwater evolution) such as rain water, glacial melt water, sea water and deep water are selected. The modelling is always relative to the selected reference waters. The modelling constraints can be changed depending on the selection of reference waters c.f. rain, snow, soil or bog water. It is important to note that the scale and the orientation of the observations in a M3-plot can change depending upon the data set used since the plot is always relative to all the other observations included in the analysis and orientated for maximum resolution. Adding or removing observations in the underlying data set can

therefore change the appearance of the plot but the internal distances between the observations are largely unchanged. The Lines are drawn between the reference waters so that a polygon is formed. The polygon defines the observations, which can be described by the selected reference waters. By definition the selected reference waters can describe the observations inside the polygon in terms of mixing and geochemical reactions.

2) *Mixing calculations* are used to calculate the mixing portions. The mixing portions describe the contribution of the reference water composition to the observed water. A calculated mixing portion can be used to indicate the origin of the groundwater. The mixing portions are equal to the distance of a sample to the selected reference waters in the M3 plot. From a two-dimensional surface, mixing portions containing a maximum of three reference waters can be calculated so that a mathematically unique solution is obtained. To avoid this shortcoming and to be able to use more than three reference waters in the model, a control point P with a known mixing portion was added to the calculations. A polygon containing, say, five reference waters contains a portion of 20% of each reference water in the centre point. By using this addition, a mathematically unique solution can be achieved from a two dimensional plane with more than three reference waters (Laaksoharju et al., 1999a). A mixing portion calculation of less than 10% is regarded as under the detection limit for the M3 method and is therefore uncertain. The overall accuracy of the model has been determined at ±10%.

3) *Mass balance* calculations are used to define the sources and sinks for different elements which deviate from the ideal mixing model used in the mixing calculations. The mixing portions are used to predict new values for the elements. No deviation from the measured value indicates that mixing can explain the element behaviour. A source or sink is due to mass balance reactions. The evolution of the groundwater can thus be described.

It is important to note that the M3 model deals only with chemical information; no space or time constraints, geological and hydrogeological information are included in the model. The calculation steps are described in more detail by Laaksoharju et al. (1999b).



Sample no	Variable 1	Variable 2	Variable 3	Variable 4	Variable 5
1	8500	45.5	19300	2.12	14.1
2	613	2.4	162	21	61
3	1960	95	93.7	234	90
4	11.5	2.3	15.4	1.9	63
5	2140	35.1	504	195	760
6	3020	7.3	4380	49.5	11
7	0	0	0	0	3
8	3179.8	154.1	152.0	379.6	146.0
9	0	0	0	2	7
10	2144	91.8	103	258	793
11	2320	26	818	217	227
12	2250	28	741	244	219
13	335	14	80	36	235
14	336	12	87	39	235
15	228	4	27	4	373

Figure 3: *Different steps in the M3 modelling; a) Data table containing groundwater compositions. b) The principle of principal component analysis; seven groundwater samples and their location in the multivariate space (VAR1-VAR5) and their projection on the principal component 1 axis (PC1) are shown. Principal component analysis is used to summarise the data information and to obtain the maximum resolution of the data set in order to construct an ideal mixing model for the site. c) The result of the principal component analysis showing principal components 1 and 2. d) Selection of possible reference waters - the other groundwater samples are compared to these, e) Mixing calculations – the linear distance of a sample to the reference waters e.g. the portions of meteoric water (%) are calculated in the figure for the selected ideal mixing model, the alternative model uses a new set of reference waters. f) Mass balance calculations – the sources and sinks (mg/l) of carbonate (HCO_3) are shown which cannot be accounted for by using the ideal mixing model and therefore the interpretation is that this is due to reactions. The M3 model is applied in this example to data from the Äspö Hard Rock Laboratory.*

5 GENERAL UNCERTAINTIES IN THE M3 MODELLING

The following errors can cause uncertainties in the M3 modelling:

1) Sampling errors caused by the effects from drilling, borehole activities, extensive pumping, hydraulic short circuiting of the borehole and uplifting (depressurization) of the water which may change the in-situ pH and Eh conditions of the sample.

2) Errors caused by inaccuracy of the analytical methods.

3) Conceptual errors such as incorrect general assumptions, selecting the wrong type/number of end-members, and mixing samples that are not mixed.

4) Methodological errors such as oversimplification and bias in the model.

Most of the errors listed above are common for many types of modelling. The effects of sampling errors are difficult to estimate since there is no in-situ sample from undisturbed conditions. By labelling drilling water, the effects from drilling can be estimated. The borehole activities and short circuiting of the borehole may cause unnatural mixing of the groundwater. In the URL the water flow is towards the shaft which decreases or eliminates this kind of contamination. The depressurization of the water can cause supersaturation of calcite which may change the Ca and HCO_3 content in the sample. The uncertainty due to sampling errors has been estimated/modelled to be of the order of ±10% from the undisturbed real values in most of the cases. Analytical errors for different elements vary but extensive comparison between different laboratories generally indicates a deviation of 1-5% in the values (Laaksoharju, 1999b).

When modelling with M3, the risk of conceptual errors occurs when making assumptions such as groundwater composition is a good tracer for the flow system (which is generally the case). The water composition may not necessarily be a unique tracer without a point source, such as labelled water in a tracer test. The accuracy is therefore much lower in M3 modelling than in a tracer test. On the other hand the temporal space is much greater and therefore the information of larger value. Another assumption in M3 is that all the reference waters are mixed. This is necessary in order to construct an ideal mixing model and to be able to compare the samples. In reality there are physical hindrances such as depth or geological structures, which may prevent mixing from occurring, and therefore not every end-member necessarily contributes to every water sample taken. Generally, three reference waters dominate in the M3 calculations and the other ones are close to or below the detection limit for the method (a mixing portion of <10%. Uncertainty can occur from selecting the wrong number and type of end-members. The selection of end-members or reference waters is a process which contains the following steps:

- Construct an independent paleo- or present-day conceptual model for the site to suggest which type of water (glacial meltwater, brine, meteoric waters) may have entered the bedrock. Here, additional information from Quaternary geology and fracture mineralogy may be helpful.

- Determine the minimum number and type of end-members needed to explain the observations using the distribution of the samples in the PCA as a guide. This is generally an iterative process where different options are tested. New end-member compositions guided by the conceptual model may be inserted in the data in order to describe the observations. The scale (e.g. fracture scale or site scale) of the modelling determines which samples are to be included in the PCA and hence the number of end-members needed for the modelling.

- Test the mixing model to see how well it predicts water conservative elements such as chloride, oxygen-18 and deuterium. Depending on the outcome of this test, the model is rejected or accepted. If rejected, the scale of modelling is changed by deleting observations and end-members. If the model is then accepted, an uncertainty range is calculated from the deviation of the water conservative elements.

- Perform a feasibility test using different mixing proportions of the reference waters to reproduce the observed groundwater composition to build confidence in the modelling. Simple tests where (say) 50% meteoric water is mixed with 50% brine water are included, to test that the water composition plots half way between the reference waters in the PCA.

Methodological errors in M3 can be due to the fact that complex groundwater compositions (which may include as many as 10 variables) are summarised by a general model where principal components 1 and 2 are used to summarise the information. The reason for using the water composition described by the 10 variables rather than constructing a model from the water conservative tracers is that it is possible to have a higher resolution in the PCA and a better chance of obtaining a unique solution. This is achieved by comparing groundwater compositions rather than that of 2 or 3 conservative tracers. As mentioned in the previous chapter the mixing calculations are mathematically unique from the 2D surface in the PCA since a centre point P allows more than 3 reference samples to be used in the calculations. The third principal component gathers generally around 10% of the groundwater information compared with the first and second principal components which contain around 70% of the information. Nevertheless, a sample may appear to be closer to a reference water in the 2D surface than in a 3D surface involving the third principal component. This can affect the accuracy of the mixing portion calculations.

In summary, the location of a sample on the PCA surface in M3 can be erroneous because of the sampling errors, analytical errors, conceptual errors and methodological errors mentioned above. These difficulties are handled in M3 by stating the uncertainty in the method as ±0.1 mixing units and the detection limit for the method as <10% of a mixing portion.

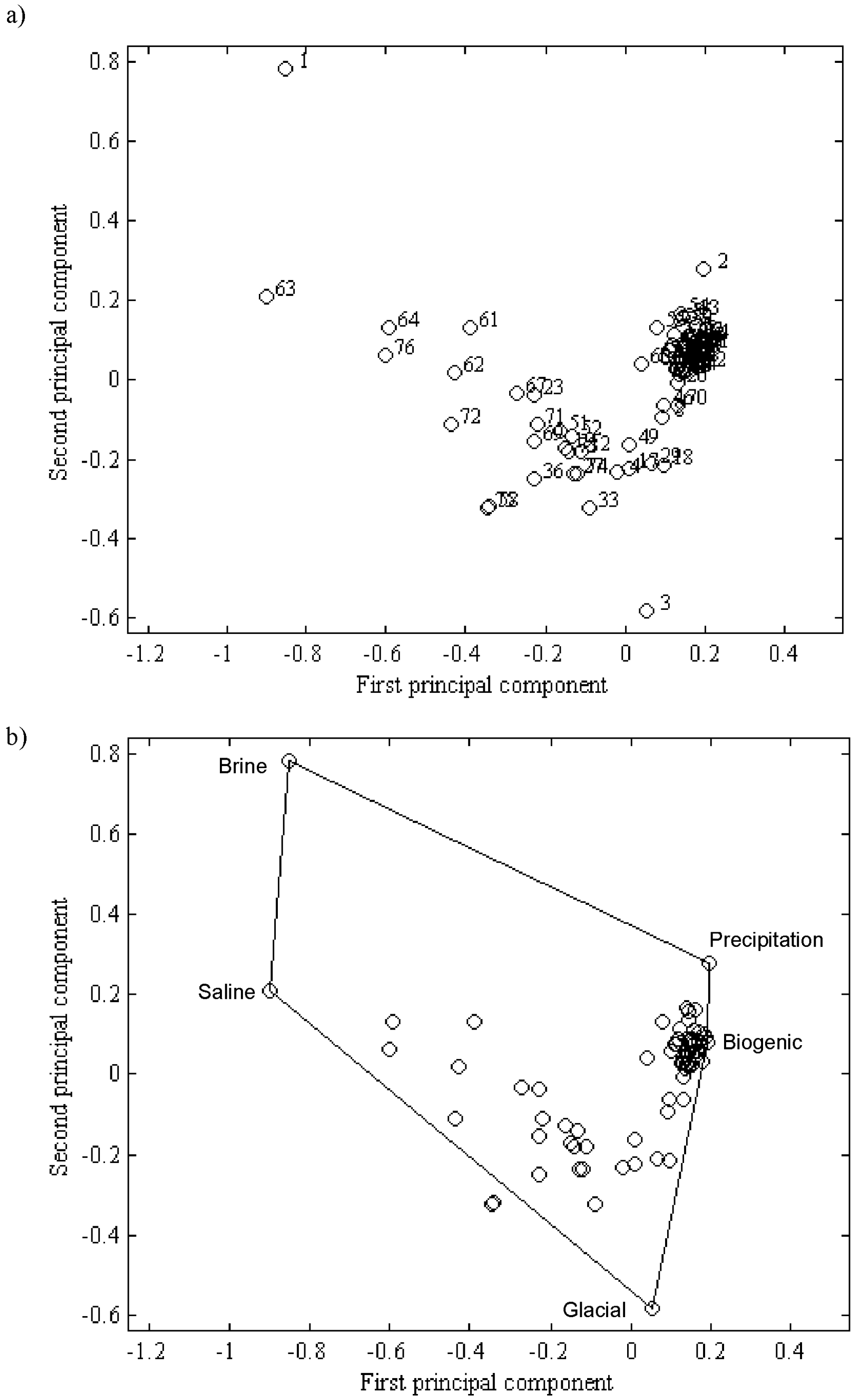
6 M3 MODELLING OF WRA DATA

In the following sections the M3 model is applied to WRA data and, principally, data from groundwaters in the area of the URL. The modelling examples show selection of reference waters, testing of the selected model, examples of reactions considered and comparison of groundwater data from Canada and Scandinavia.

6.1 Selection of reference waters

In order to select reference waters for WRA data in M3 modelling the variables Na, K, Ca, Mg, Cl, SO_4 HCO_3, δ^2H, ^3H and $\delta^{18}O$ were used in a principal component analysis. The results of the principal component analysis are shown in Figure 4a, b.

a)



PC 1 = – 0.39[Na] + 0.03[K] + 0.25[Ca] + 0.09[Mg] – 0.39[HCO3] + 0.62[Cl] + 0.18[SO4] + 0.32[18O] + 0.22[2H] – 0.24[3H]

PC 2 = – 0.45[Na] + 0.12[K] + 0.07[Ca] + 0.04[Mg] – 0.02[HCO3] + 0.11[Cl] – 0.16[SO4] – 0.85[18O] + 0.14[2H] + 0.02[3H]

Figure 4: **a)** *The Principal Component plot based on the major components and water conservative tracers Cl, deuterium, O^{18} and tritium. The numbers refer to groundwater samples listed in Appendix 1.* **b)** *The reference waters Precipitation, Biogenic, Glacial, Saline and Brine have been selected from the data set used in the principal component analysis. A polygon is drawn between the samples in order to define the samples that can be described by the ideal mixing model. The equations for the first (PC1) and second (PC2) principal component describe the loadings from the different elements in the model. The first and second principal components together describe 67% of the variability or the information of the groundwater samples.*

The selected reference waters for the current modelling are (analytical data are listed in Appendix 1):

- **Brine reference water** representing the brine type of water (Ca-Cl in composition) found in the rock matrix (Cl = 53,300 mg/l, Gascoyne et al. 1996).
- **Saline reference water** which represents saline groundwater (Na-Ca-Cl in composition) found at depth in fracture zones in the WRA (Cl = 30,200 mg/l). This type of water is found in borehole WB1-7 (Gascoyne, 2000).
- **Glacial reference water** which has been determined as a glacial water with a assumed stable isotope value ($\delta^{18}O$ = -25‰ SMOW) which indicate cold climate recharge (Gascoyne, 2000).
- **Biogenic reference water** which represents water found in the borehole M12-159 possibly altered by bacterial decomposition of organic material coupled with high CO_2 production in combination with uptake near the surface. The water is characterised by a high content of HCO_3 (255mg/l) but a rather low content of Ca (6.5 mg/l) which suggest a contribution from organic decomposition rather than calcite dissolution.
- **Precipitation reference water** which represents a dilute infiltrating surface water affected by the precipitation from the 1960's and therefore contains more tritium (^3H = 90 TU) than modern rain (~20 TU).

6.2 Test of selected model

In the M3 modelling, selected reference waters are tested before an optimum model for the site is chosen. Since M3 only compares groundwater samples at a site, the selection of reference waters determines what type of modelling is to be performed and at what scale. If only shallow groundwater is modelled, then there is no need to include brine as a reference water, but if the aim is to investigate the geochemical relationship between deeper waters and brine, a brine water composition has to be included in the modelling. The internal similarities/dissimilarities and the distribution of the samples in the principal component analysis generally help to select the appropriate number and types of reference waters for M3 modelling. In any case, this generally requires several M3 runs where models using different types and numbers of reference waters are tested. The criteria for a feasible model for a site is:

- The model can describe as many groundwater samples as possible
- The mixing calculations are in general agreement with the hydrogeological description of the groundwater and the conceptual/evolutionary model of the site
- The deviations for the conservative constituents are reasonable
- The deviations for the non-conservative elements make geochemical sense

In the example in Figure 5 the calculated values for WRA data are compared with measured values for different groundwater constituents. If the value is on the line the predicted and measured value, coincide; if the value is above/under the line there is a deviation between the measured and predicted value. A deviation from the line for the water conservative constituents such as Cl, oxygen-18 ($\delta^{18}O$) and deuterium ($\delta^{2}H$) indicates scatter in the model. A deviation for a reactive element such as HCO_3 can indicate gain (values over the line) or losses (values under the line) associated with reactions. The results in Figure 5 can be used to check the feasibility of the selected model for the site.

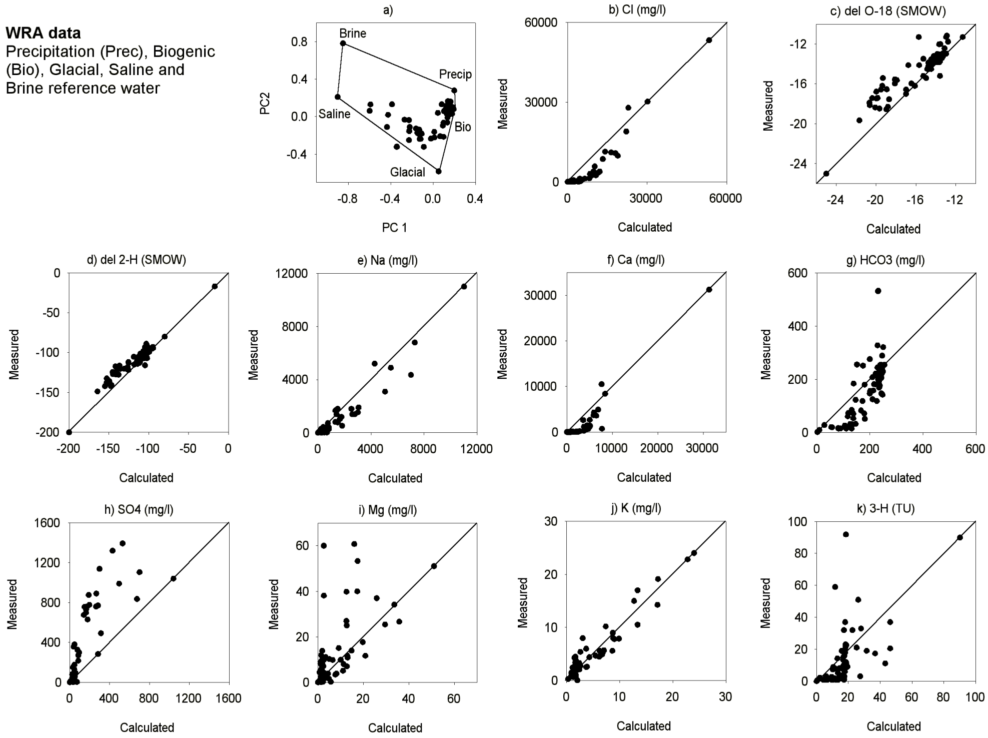


Figure 5*: The WRA groundwaters are modelled to be a mixture of Precipitation, Biogenic, Glacial, Saline and Brine type of water as shown in the PCA (Figure a). The model can describe the water conservative elements (Cl, $\delta^{18}O$, $\delta^{2}H$) fairly well (note the different scales in Figures b, c and d) and most of the observations are included in the model (inside the polygon). A deviation for a reactive element such as Na, Ca, HCO_3, SO_4, Mg and K can indicate gain (values over the line) or loss (values under the line) associated with water rock interactions. The gain of tritium (^{3}H) shows that some of the observations have a higher tritium content (older water from nuclear testing) than the selected reference water (Precipitation). The loss of tritium for some samples can indicate radioactive decay.*

6.3 Reactions considered

In theory thousands of chemical reactions could be written involving the water, solids and gases in regional aquifers such as those at the URL site. There are eight main categories of reactions and processes that control the chemistry of most groundwaters: precipitation-dissolution, acid-base, complexation, substitution-hydrolysis, oxidation-reduction, ion-filtration-osmosis, dissolution and exsolution of gases and sorption/desorption. Worldwide site modelling has revealed that the actual number of reactions that dominate the groundwater chemistry is quite small (Alley, ed., 1993) such as:

1) Introduction of CO_2 gas in the unsaturated zone
2) Dissolution of calcite and dolomite, and precipitation of calcite
3) Cation exchange
4) Oxidation of pyrite and organic matter
5) Reduction of oxygen, nitrate, and sulphate, with production of sulphide
6) Reductive production of methane
7) Dissolution of gypsum, anhydrite and halite
8) Incongruent dissolution of primary silicates with formation of clays

In theory any effect from an inorganic/organic reaction can be traced by using M3. In practice the selection of reference waters, the validity of the ideal mixing model, model errors and the fact that a gain or a loss of an element can be due to several different reactions give constraints on what kind of reactions can be traced with any accuracy. The M3 modelling is always relative to the selected reference waters and therefore describes always and only the *net* reactions which have to take place if these waters are mixed. The *total* reactions are the net reactions plus the reactions which have to take place to form the reference water (eg. Brine water).

Since much of the URL modelling in this work aimed at describing the groundwater situation affected by the shaft construction this added an important constraint in the modelling, namely to focus on the fast short-term reactions in the modelling. The relatively low temperature of the groundwater often hinders equilibrium from being established between the groundwater and fracture minerals. Instead, recent research (eg, Pedersen and Karlsson, 1995; Stroes-Gascoyne and Gascoyne, 1998,) has shown that microbes mediate in many reactions that otherwise would not take place. Organic material (CH_2O) generally plays an important role in these kinds of biogenic processes. The processes that are of major influence on the obtained groundwater at the URL site are biological processes, redox reactions, calcite dissolution/precipitation and ion exchange. As an example, the effects from the following major reactions can be modelled in detail with the M3 code:

1) **Organic decomposition:** This reaction is generally detected in the unsaturated zone associated with infiltrating precipitation water. This process consumes oxygen and adds reducing capacity to the groundwater according to the reaction: $O_2 + CH_2O \rightarrow CO_2 + H_2O$. M3 reports a gain of HCO_3 as a result of this reaction.

2) **Organic redox reactions:** An important redox reaction is reduction of iron III minerals through oxidation of organic matter: $4Fe(III) + CH_2O + H_2O \rightarrow 4Fe^{2+} + 4H^+ + CO_2$. M3 reports a gain of HCO_3 as a result of this reaction (this reaction was not modelled for the WRA data). This reaction takes place in the shallow part of the bedrock associated with influx of precipitation water.

3) **Inorganic redox reaction:** An example of an important inorganic redox reaction is sulphide oxidation in the soil and of the fracture minerals containing pyrite according to the reaction: $HS^- + 2O_2 \rightarrow SO_4^{2-} + H^+$. M3 reports a gain of SO_4 as a result of this reaction. This reaction generally takes place in the shallow part of the bedrock or in the case of a drawdown such as in the URL, at larger depths.

4) **Dissolution and precipitation of calcite:** There is generally a dissolution of calcite in the upper part and precipitation in the lower part of the bedrock according to the reaction: $CO_2 + CaCO_3 \rightarrow Ca^{2+} + 2HCO_3^-$. M3 reports both gains and losses of Ca and HCO_3 as a result of this reaction. This reaction can take place in any groundwater type.

5) **Ion exchange:** Cation exchange with Na/Ca is a common reaction in groundwater according to the reaction: $Na_2X_{(s)} + Ca^{2+} \rightarrow CaX_{(s)} + 2Na^+$, where X is a solid substrate such as a clay mineral. M3 reports a change in the Na/Ca ratios as a result of this reaction. This reaction can take place in any groundwater type.

6) **Sulphate reduction:** Microbes can reduce sulphate to sulphide using organic substances in natural groundwater as reducing agents (Laaksoharju ed., 1995) according to the reaction: $SO_4^{2-} + 2CH_2O + OH^- \rightarrow HS^- + 2HCO_3^- + H_2O$. This reaction is of importance since it may cause corrosion of copper canisters used in the final storage. Vigorous sulphate reduction is generally detected in association with marine sediments that provide the organic material and the favourable salinity interval for the microbes. M3 reports a loss of SO_4 and a gain of HCO_3 as a result of this reaction. This reaction modifies the groundwater composition by increasing the HCO_3 content and decreasing the SO_4 content. At the URL, this reaction does not occur.

Of the above reactions only the reaction associated with organic decomposition (reaction#1) was modelled in this work (see section 7.3).

6.4 Comparison of groundwater data

M3 can be used for explorative data analysis where large data sets are examined. In this modelling example the WRA data is compared by using principal component analysis in M3 with all the deep groundwater sampled in crystalline bedrock in Sweden and Finland (Figure 6). Groundwater samples which plot close to each other in the plot have a similar groundwater composition. A sample which plots close to one representing precipitation is therefore assumed to contain more rain water or snow-melt than a sample which plots close to one representing a brine type of water. The results show that WRA data is similar to the shallow water (precipitation, and biogenic water (a water type affected by organic reactions)) but is more affected by cold recharge water (glacial water) than seen in the Scandinavian data. The brine water is different from the Scandinavian brine sample and not surprisingly, marine water has not affected the WRA data to any large extent.

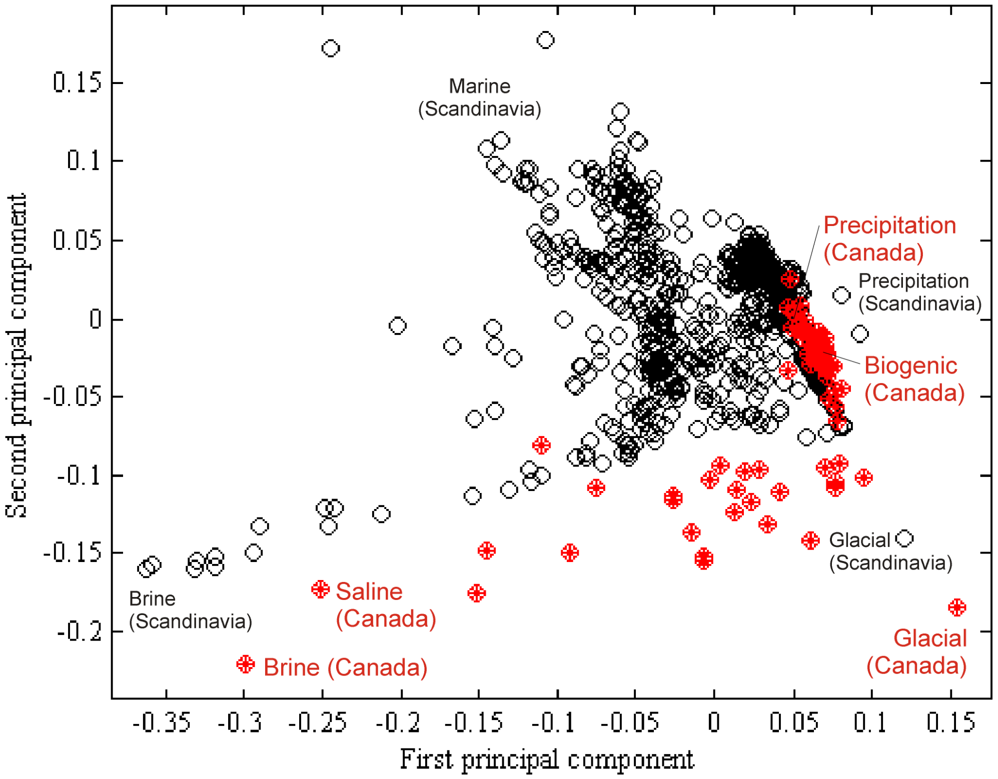


Figure 6: *Principal component analysis in M3 is used to compare groundwater samples from Scandinavia (Sweden and Finland) with Canadian WRA data. The Canadian data are included in a principal component analysis together with Scandinavian data. The modelling is based on the major components, stable isotopes and tritium values in more than one thousand samples. Samples with a similar groundwater composition tend to form clusters in the plot. In order to help the comparison some extreme waters (end-members) such as marine water (sea water), precipitation (rain water), biogenic water (water affected by organic decomposition resulting in* CO_2 *production and uptake), glacial water (cold recharge water from the last de-glaciation) and brine water (old saline water affected by long term water rock interactions with the rock matrix. The two principal components together account for 65% of the variability, of the information in the data set.*

7 VISUALISATION OF M3 MODELLING RESULTS

The measured values and the results from the M3 modelling can be illustrated as contour plots for the site (Figures 7-15). These plots are based on 2D KRIGING interpolations using the computer code SURFER®. The 2D interpolation in a NNW-SSE direction was based on a total of 20 groundwater samples at the URL site. To reduce uncertainties, the cross-section was chosen where most of the sampling points were located. The samples are numbered in Figures according to observation number in Appendix 1.

The interpolation is uncertain at large depths (>500m) and in the corners of the cross-section where there are few or no observations. It is important to note that the water is flowing in fractures, but since there is a fracture network at the URL and, at large scale, the groundwater can mix, an interpolation method can be employed. The results of the interpolation should be regarded as a potential map for a certain groundwater property to occur at a given bedrock location. The map has a high degree of accuracy only close to the sampling points.

7.1 Water conservative tracers

The interpolated distribution of measured Cl and $\delta^{18}O$ content is shown as cross-sections in Figures 7 and 8. Figure 7 shows that the chloride content is increasing with depth and towards the NNW. The Cl distribution may give the impression that the groundwater system is fairly simple and can be described mostly as following a two component evolutional path between non-saline and saline groundwater. The oxygen-18 content is decreasing in the NNW part of the model which indicates effects from cold recharge that is now present in this part of the bedrock (Figure 8). A more detailed evaluation of these known groundwater conservative tracers shows that the correlation is not always high (c.f. Figure 3) which may indicate a more complex groundwater system than can be assumed from the Cl distribution.

The reason for the low correlation between Cl and $\delta^{18}O$ is that waters with the same Cl content may have different origins. For example, a water containing the same Cl content could have been affected by waters with different recharge temperatures and therefore a different origin. The groundwater mixing results in ambiguous groundwater signatures and difficulties in understanding and modelling the site if only one variable is used as a tracer for the transport of constituents.

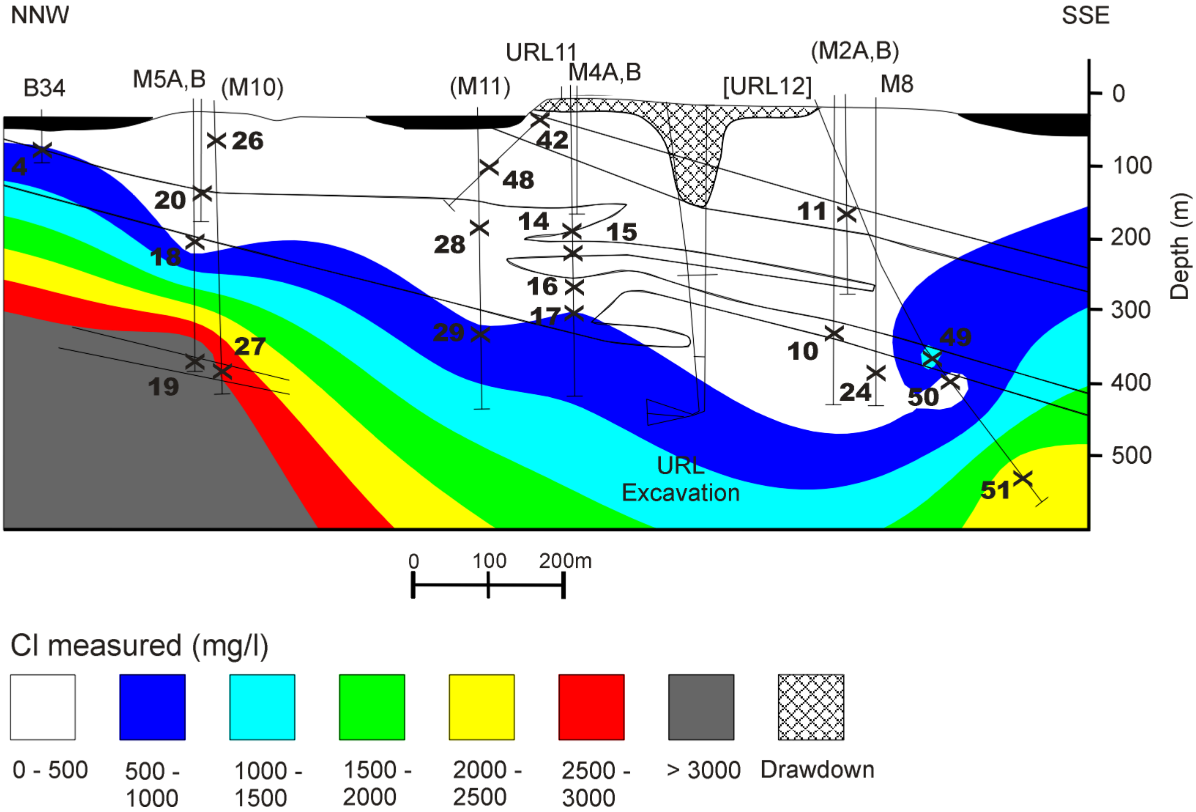


Figure 7: *Visualisation of the measured Cl distribution at the URL site. The chloride content seems to be increasing with depth and towards NNW. The approximate associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

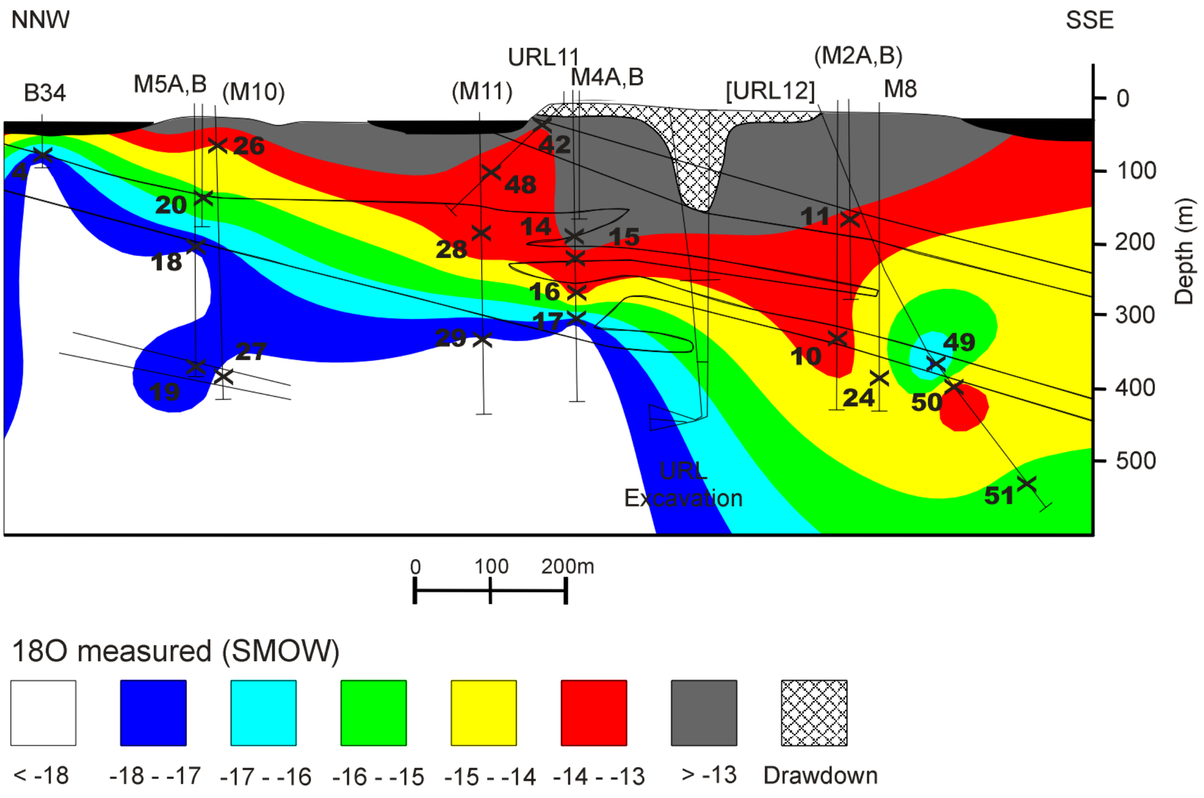


Figure 8: *Visualisation of the measured* $\delta^{18}O$ *distribution at the URL site. The oxygen-18 content is decreasing in the NNW part of the model which may indicate effects from cold recharge now present in this part of the bedrock. The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

7.2 Mixing proportions

The results of M3 mixing calculations are shown as 2D cross-sections in Figures 9-13 for the water types: precipitation, biogenic, glacial, saline and brine. The mixing portions always add up to 100% for all the samples. The construction of the URL created a large drawdown of the groundwater table around the elevator shaft. The drawdown resulted in changing inflow patterns and probably increased the mixing of different groundwater types.

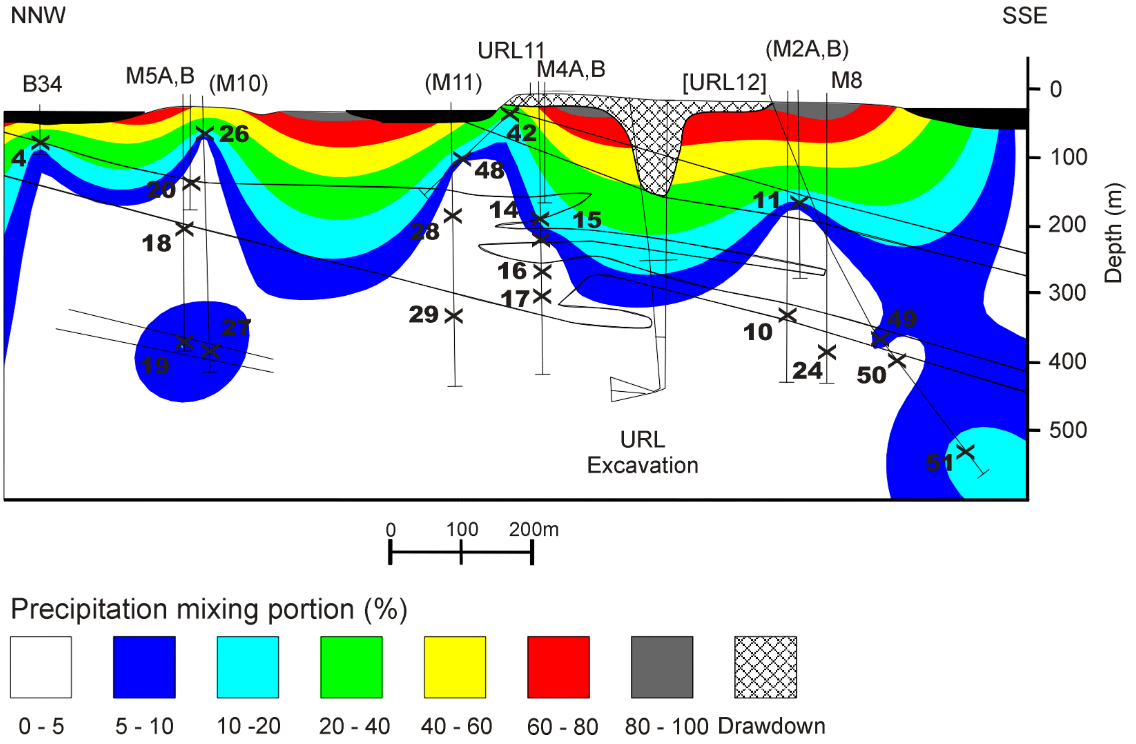


Figure 9: *Visualisation of the M3 calculated proportion (%) of precipitation water in the bedrock at the URL site. The precipitation water content is high at the surface and generally decreases with depth. The content of 5-20% of precipitation water at large depths in the boreholes M5A, M10 and URL 12 could be due to borehole activities (e.g. presence of residual drill-water). The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

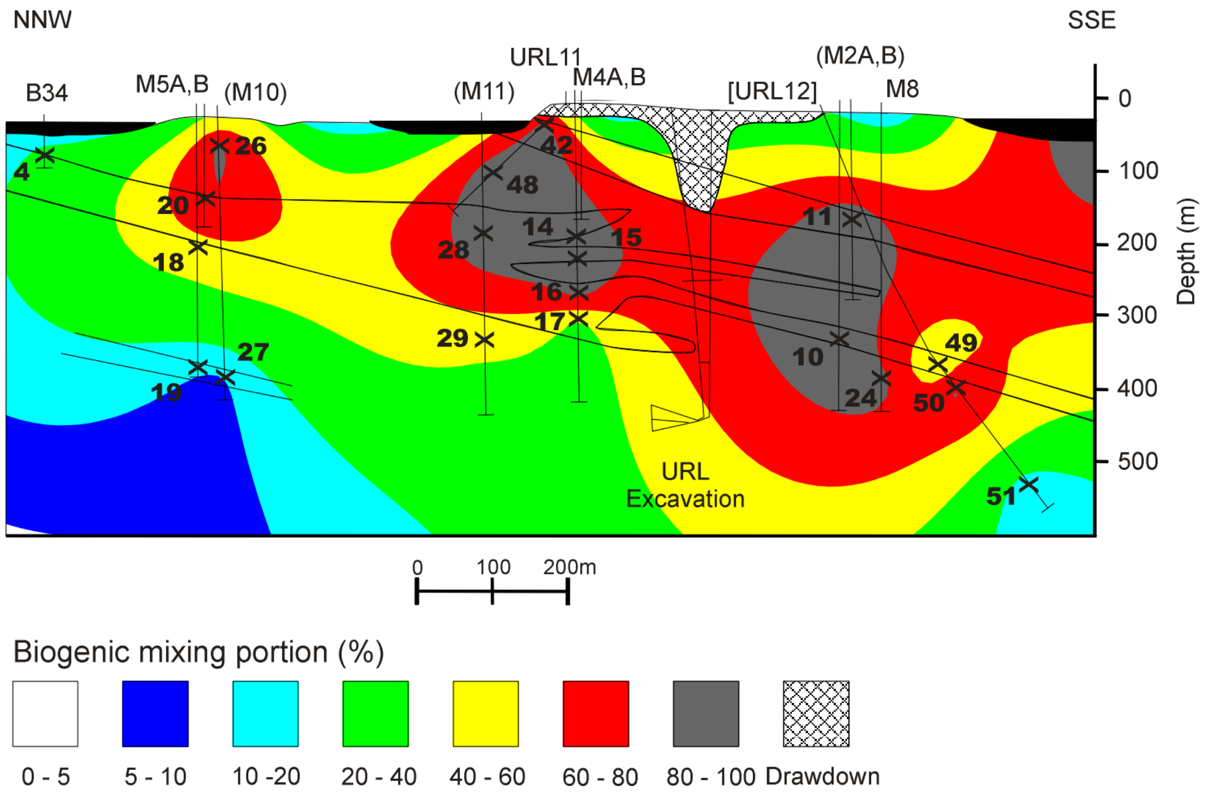


Figure 10: *Visualisation of the M3 calculated proportion (%) of biogenic water in the bedrock at the URL site. The biogenic water content is high in the upper part of the bedrock to a depth of 200m but also appears to exist at a greater depth (400m) close to the shaft. This water type is mainly affected by decomposition of organic material and uptake of* CO_2 *in the overburden which adds reducing capacity to the groundwater. The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

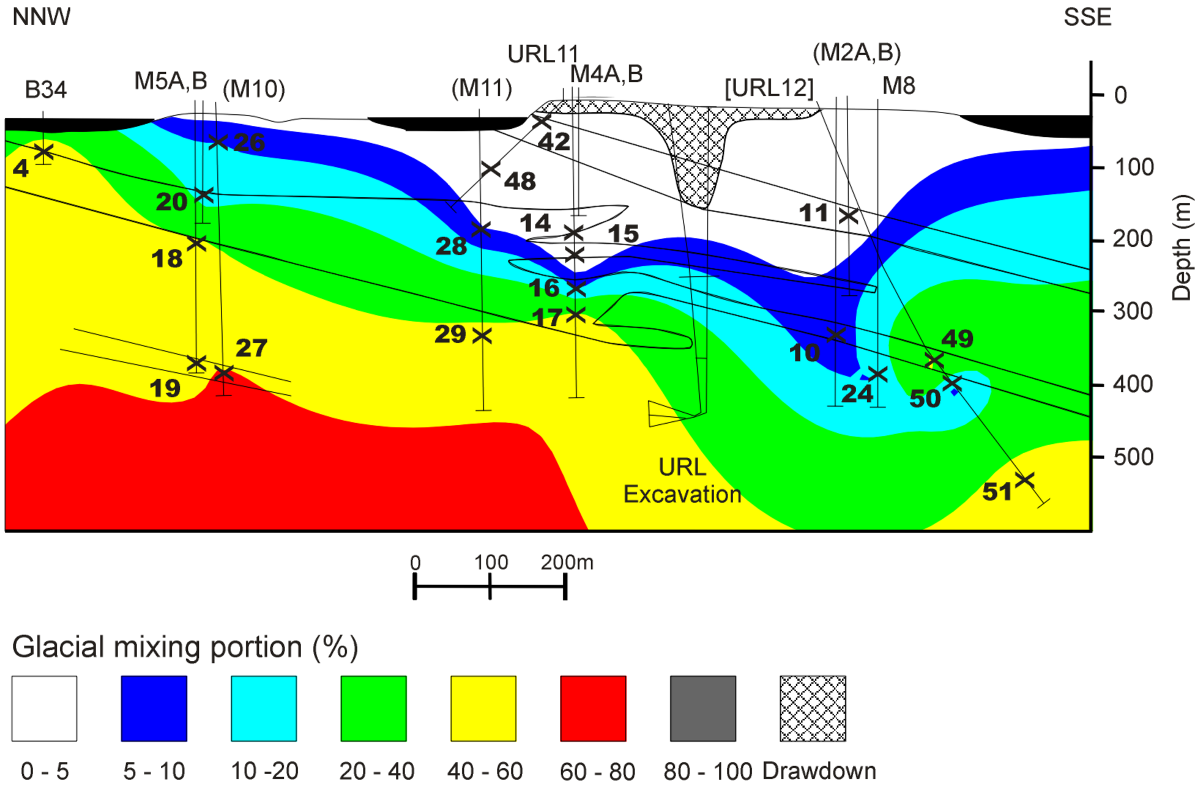


Figure 11: *Visualisation of the M3 calculated proportion (%) of glacial water in the bedrock at the URL site. The glacial water content is high in the NNW part of the bedrock at larger depths than 400m. This water type is mainly affected by cold meltwater from the last deglaciation which lowers the oxygen-18 content. The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

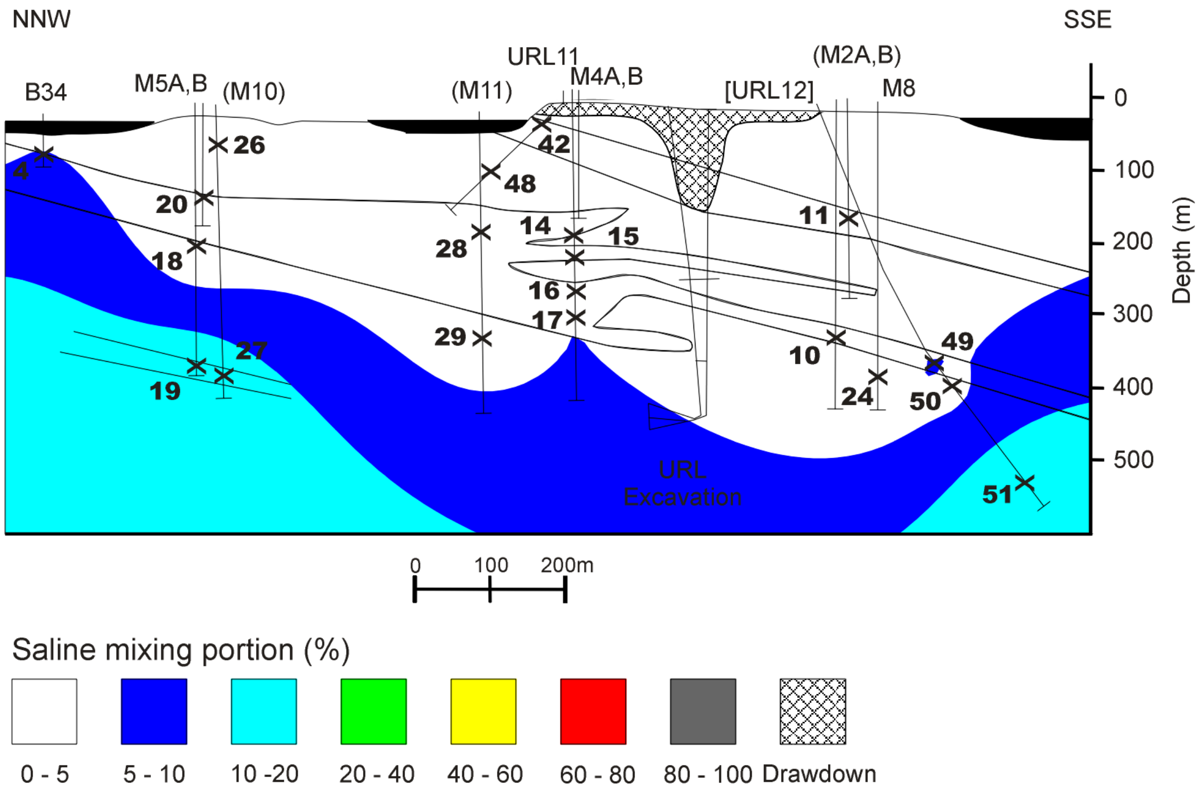


Figure 12: *Visualisation of the M3 calculated proportion (%) of saline water in the bedrock at the URL site. The saline water content increase in the NNW and the SSE part of the bedrock at greater depths than 300m. This water type is mainly affected by long term water rock interactions and is regarded as being pre-glacial. The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

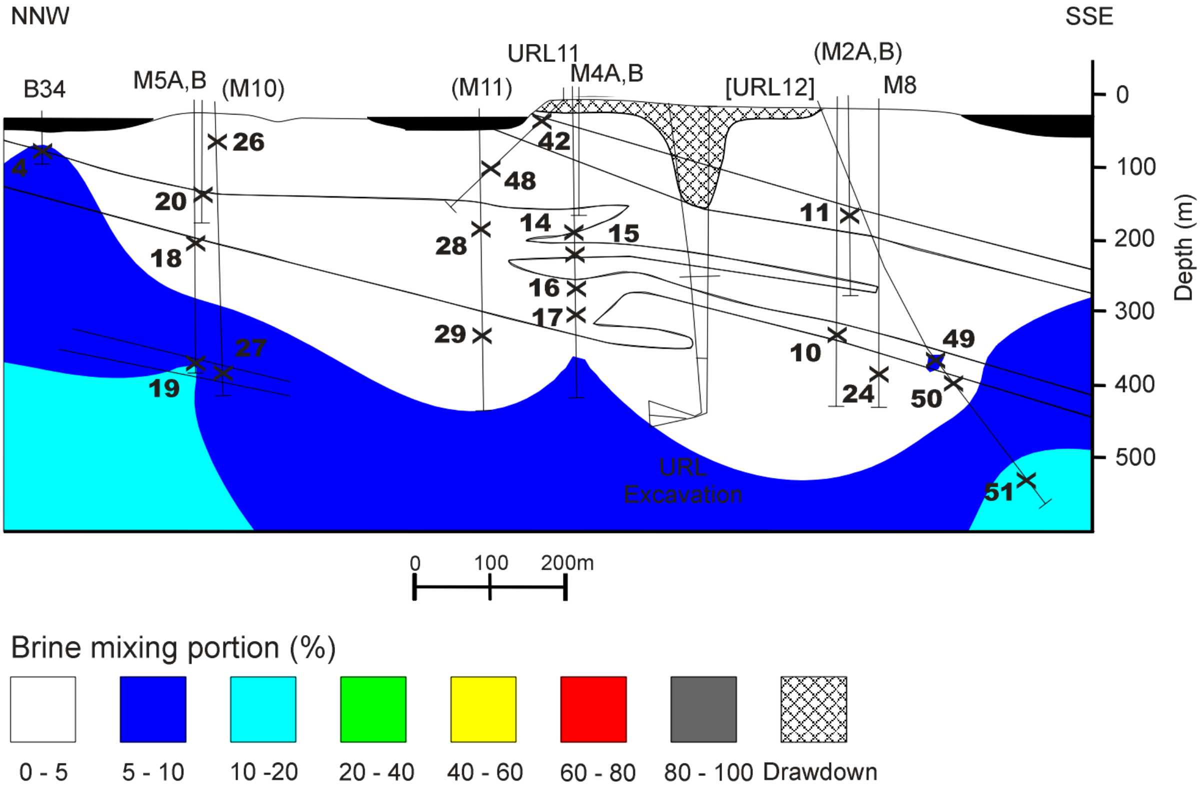


Figure 13: *Visualisation of the M3 calculated proportion (%) of brine water in the bedrock at the URL site. The brine water content increases in the NNW and the SSE part of the bedrock at greater depths than 300m. This water type is similar to that of the saline groundwater (Figure 12) except for the dominance of Ca, and may contribute to the salinity content in the saline groundwater. The high salinity of brine water is affected by long term interactions with the rock matrix. The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

The results of the M3 mixing calculations shown in Figures 9-13 indicate that the upper part of the bedrock (0-100m) is dominated by precipitation type of water (100-40%). At greater depths (100-400m) the precipitation water is replaced by biogenic water (40-100%) which gradually consumes the oxygen of the groundwater, thus becoming reducing. At the depths of 300-600m and in the NNW part of the bedrock glacial water (40-80%) from the last deglaciation dominates. In the NNW and SSE part and at the same depth interval as the glacial water (300-600m), the influence of saline (5-20%) and brine (5-20%) types of water is detected. The draw-down from the shaft increased the portions of precipitation and biogenic water but seems to have flushed out historical waters such as glacial, saline and brine and hence the proportion of these waters were low around the shaft. The occurrence and the distribution of water types are in good agreement with earlier groundwater modelling of the site (e.g., Gascoyne, 1997).

7.3 Mass-balance calculations

An example of results from the M3 mass-balance calculations is the behaviour of the carbonate system at the URL site. Input of organic carbon into shallow groundwater provides a possible energy and carbon source for anaerobic respiration (see section 6.4). The measured HCO_3 content and the calculated M3 deviation for this element is shown in Figures 14 and 15. The modelling indicates that there is a gain of HCO_3 not accounted for by mixing mainly associated with organic decomposition in the biogenic water type and the enrichment of CO_2 in near-surface sediments. At larger depths and in the NNW part of the site the modelling indicates a loss which may be due to calcite precipitation. The mass-balance modelling for the carbonate system is in good agreement with earlier groundwater modelling of the site (e.g., Gascoyne, 1997). The complete M3 mass-balance modelling results for all the elements are reported in Appendix 1.

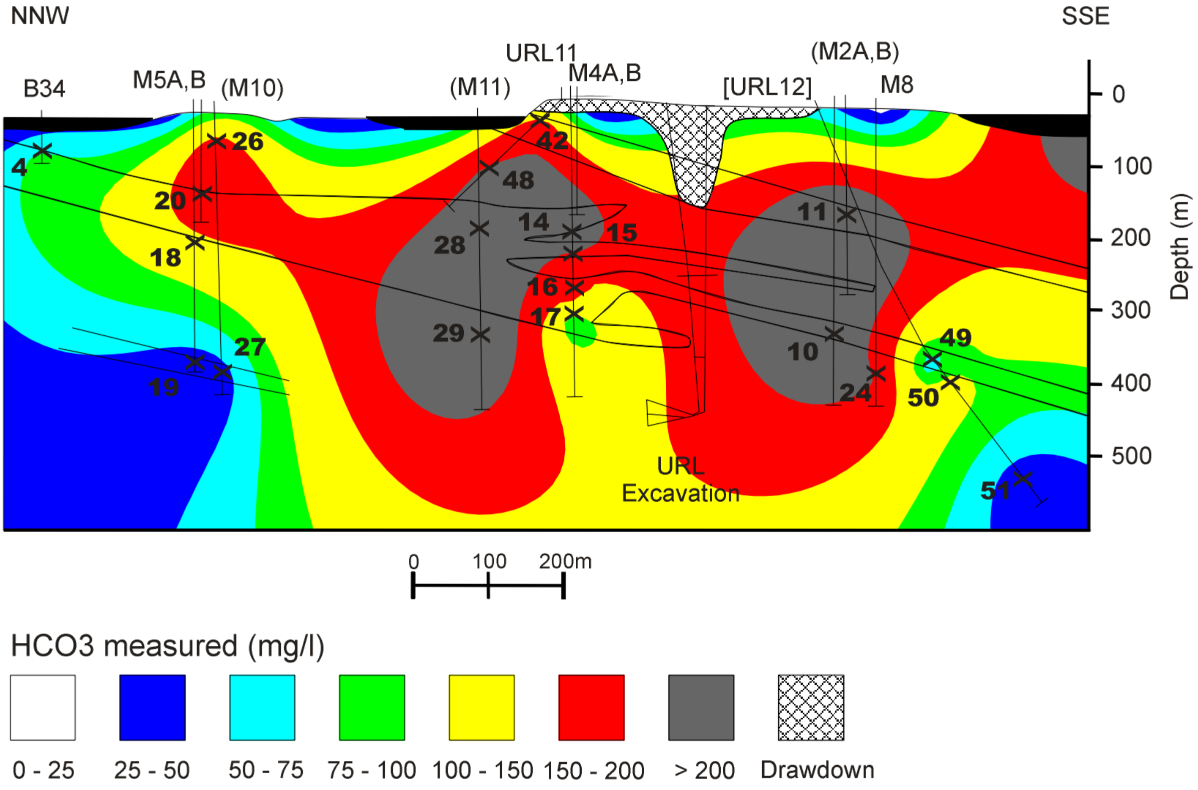


Figure 14: *Visualisation of the measured HCO_3 content at the URL site. High concentrations are detected at the depths 100-400m close to the URL shaft. The HCO_3 content correlates with the biogenic water type (c.f. Figure 10). The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations is shown.*

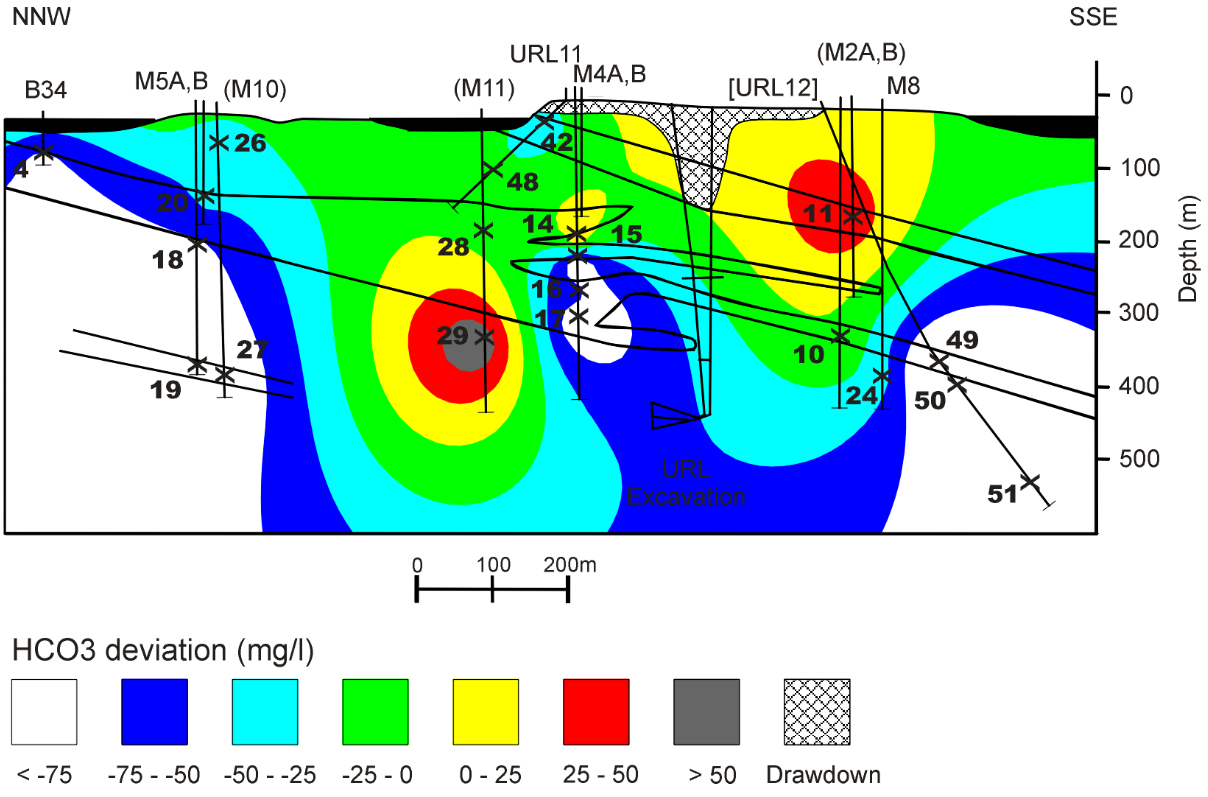


Figure 15: *Visualisation of the M3 mass-balance calculations indicate a gain (positive value) of HCO_3 not accounted for by mixing. The gain correlates with the biogenic water type (c.f. Figure 10) and can be due to organic decomposition. At larger depths and in the NNW part of the bedrock the modelling indicates a loss (negative value) which can indicate calcite precipitation. The approximate drawdown associated with the shaft construction, the major fracture zones, boreholes and sampling locations are shown.*

8 CONCLUSIONS

M3 modelling was applied to WRA hydrogeochemical data in order to determine its potential as a modelling tool in the site description and evaluation process. The aim was not to perform a complete modelling of the WRA but rather to demonstrate if some of the results from previous work at the URL site could be repeated by using this new approach.

In M3 modelling the assumption is that the groundwater chemistry is a result of mixing as well as water/rock reactions. The M3 model compares the groundwater compositions from a site. The similarities and differences of the groundwater compositions are used to quantify the contribution from mixing and reactions on the measured data. In order to construct a reliable model, the method is used to summarise the information from the groundwater data set by using the major components Cl, Ca, Na, Mg, K, SO_4 and HCO_3 in combination with the isotopes δ^2H, $\delta^{18}O$ and ^3H. Initially, the method quantifies the contribution from the flow system by comparing groundwater compositions to identified reference waters. Subsequently, contributions from reactions are calculated. The model differs from many other standard models, which primarily use reactions rather than mixing, to determine the groundwater evolution. The uncertainty in the method is ±0.1 mixing units and the detection limit for the method is <10% of a mixing portion.

The modelled present-day groundwater conditions at the URL site consist of a mixture in varying degrees of the following water types: precipitation, biogenic, glacial, saline and brine. The results of the M3 mixing calculations indicate that the upper part of the bedrock (0-100m) is dominated by precipitation type of water (100-40%). At greater depths (100-400m) the precipitation water is replaced by biogenic water (40-100%) which gradually consumes the oxygen of the groundwater and becomes reducing. At depths 300-600m and in the NNW part of the bedrock glacial water (40-80%) from the last deglaciation dominates. In the NNW and SSE part and at the same depth interval as the glacial water (300-600m) the influences from saline (5-20%) and brine (5-20%) type of waters are detected. The glacial water is a relatively thin lens and is underlain by the saline, warm-climate water typical of WB 1-7 at ~1000m depth. The draw-down from the shaft increases the portions of precipitation and biogenic water but seemed to have flushed out historical waters such as glacial, saline and brine from the near vicinity of the shaft. The M3 mass-balance modelling indicates that there is a gain of HCO_3 not accounted for by mixing probably associated with organic decomposition and CO_2 uptake in the biogenic water type . At larger depths and in the NNW part of the bedrock, the modelling indicates a loss which may be due to calcite precipitation. The occurrence and the distribution of water types and the mass-balance calculations for carbonate are in general agreement with earlier groundwater modelling of the site.

Although the M3 model is fairly new, with relatively few test cases, and requires complex multivariate mathematics, the major advantages of the model are:

- It is a mathematical tool which can be used to evaluate groundwater field data and to support expert judgement of a site.
- The tool is not dependent on thermodynamic databases and can handle effects of biogenic reactions
- The results of mixing calculations can be compared/integrated with hydrodynamic models
- The numerical results of the modelling can be visualised and presented for non-expert use.

9 ACKNOWLEDGEMENTS

This study has been financed by Ontario Power Generation (OPG) and the Swedish Nuclear Fuel and Waste Management Company (SKB). The support from Mark Jensen (OPG) and Peter Wikberg (SKB) are acknowledged.

10 REFERENCES

AECL 1994. Environmental Impact Statement on the Concept for Disposal of Canada's Nuclear Fuel Waste. Atomic Energy of Canada Limited Report AECL-10711/COG-93-1.

Alley W M (ed.), 1993. Regional groundwater quality. ISBN 0-442-00937-2. Van Nostrand Reinhold, New York, USA, pp634.

Gascoyne, M. 2000. Hydrogeochemistry of the Whiteshell Research Area. Ontario Power Generation Report, in press.

Gascoyne M 1997 Evolution of Redox Conditions and Groundwater Composition in Recharge-Discharge Environments on the Canadian Shield, Hydrogeology Journal, Vol. 5, No. 3, 1997. Alley W M (ed.), 1993. Regional groundwater quality. ISBN 0-442-00937-2. Van Nostrand Reinhold, New York, USA, pp634

Gascoyne, M., A. Bath and A. Gautschi. 1991. Hydrogeochemical monitoring requirements for radioactive waste disposal in geological environments. In: Long Term Observations of the Geological Environment: Needs and Techniques, Proc. OECD/NEA Conf., Helsinki, Finland, 1991 September 9-11, 93-108.

Gascoyne M and Thomas D, 1997, Impact of blasting on groundwater composition in a fracture in Canada's Underground Research Laboratory, Journal of Geophysical Research, Vol. 102, No. B1, pages 573-584, 1997.

Gascoyne M, Frost L, Haveman S, Stroes-Gascoyne S, Thorne G, Vilks P, Clarke D, Ross J, Watson R, 1997, Chemical Evolution of Rapidly Recharging Groundwaters in Shield Environments, AECL-11814, COG-97-264-I.

Gascoyne, M., R.D. Ross and R.L. Watson. 1996. Highly saline pore fluids in the rock matrix of a granitic batholith on the Canadian Shield. Abstract of paper presented at International Geological Congress, Beijing, China, Aug. 4-14, 1996

Gascoyne M, 1996, The geochemical environment of nuclear fuel waste disposal. Canadian Journal of Microbiology, Vol. 42, No. 4, pages 401-409, 1996.

Gascoyne M and Wuschke D, 1996, Gas migration through water-saturated, fractured rock: results of a gas injection test, Journal of Hydrology 196 (1997) pages 76-98.

Gascoyne M, 1994, Isotopic and geochemical evidence for old groundwaters in a granite on the Canadian Shield: Radiochemical Acta, v. 58/59, p. 281-284.

Gascoyne M and Chan T, 1992, Comparision of numerically modelled groundwater residence time with isotopic age data, in Paleohydrogeological methods and their applications, Nuclear Energy Agency Workshop, 1992, Paris France: Proceedings, NEA/OECD, p. 199-206..

Gurban I, Laaksoharju M, Ledoux E, Made B, Salignac AL, 1998. Indications of uranium transport around the reactor zone at Bagombé (Oklo). SKB Technical Report TR-98-06, Stockholm, Sweden.

Kotzer T, Gascoyne M, Mukai M, Ross J, Waito G, Milton G, Cornett R, 1998, ^{36}*Cl,* ^{129}*I and Noble Gas Isotope Systematics in Groundwaters from the Lac du Bonnet Batholith, Manitoba, Canada. Radiochim. Acta 82, pages 313-318, 1998.*

Laaksoharju M, Skårman C, Skårman E, 1999a. Multivariate Mixing and Mass-balance (M3) calculations, a new tool for decoding hydrogeochemical information. Applied Geochemistry Vol. 14, #7, 1999, Elsevier Science Ltd., pp861-871.

Laaksoharju M, Tullborg E-L, Wikberg P, Wallin B, Smellie J, 1999b. Hydrogeochemical conditions and evolution at Äspö HRL, Sweden. Applied Geochemistry Vol. 14, #7, 1999, Elsevier Science Ltd., pp835-859.

Laaksoharju M, Gurban I, Andersson C, 1999c. Indications of the origin and evolution of the groundwater at Palmottu. The Palmottu Natural Analogue Project. SKB Technical Report TR 99-03, Stockholm, Sweden.

Laaksoharju, M; Wallin, B (eds.) 1997. Evolution of the groundwater chemistry at the Äspö Hard Rock Laboratory. Proceeding s of the second Äspö International Geochemistry Workshop, June 6-7, 1995. SKB HRL International Cooperation Report ICR 97-04. Laaksoharju, M (ed.), Gustafson G, Pedersen K, Rhén I, Skårman C, Tullborg E-L, Wallin B, Wikberg P, 1995. Sulphate reduction in the Äspö HRL tunnel. SKB Technical Report TR 95-25, Stockholm, Sweden.

Pedersen K, Karlsson F, 1995. Investigation of subterranean bacteria - Their importance for performance assessment of radioactive waste disposal. In: SKB Technical Report TR 95-10, Stockholm, Sweden.

Stroes-Gascoyne S and Gascoyne M, 1998, The Introduction of Microbial Nutrients into A Nuclear Waste Disposal Vault during Excavation and Operation. Environmental Science & Technology, Vol. 32, No. 3, pages 317-326, 1998.

11 APPENDIX 1

Appendix 1 shows the WRA-data used in M3 modelling. The results from the M3 mixing and mass-balance (deviation) calculations are listed. The numbers in the first column represent the row numbers used as index numbers in M3 modelling. Items in **bold** indicate the reference waters used in the different M3 calculations. Grey shaded cells mark samples used for interpolation/visualization (Kriging). Italics indicates samples used as boundaries for the interpolations.

	Sample name	Date	Measured Na (mg/l)	Measured K (mg/l)	Measured Ca (mg/l)	Measured Mg (mg/l)	Measured HCO3 (mg/l)	Measured Cl (mg/l)	Measured SO4 (mg/l)	Measured 18O (SMOW)	Measured 2H (SMOW)	Measured 3H (TU)
1			**1410**	**22.8**	**31270**	**0.118**	**28**	**53300**	**284**	**-17**	**-17**	**0.8**
2			**0.29**	**0.31**	**0.55**	**0.085**	**1.85**	**0.44**	**1.09**	**-11.3**	**-80**	**90**
3			**20**	**2**	**35**	**10**	**180**	**2**	**15**	**-25**	**-200**	**0**
4	B34-2	28-Jul-88	410	4.4	85	15.1	82.86	595.3	300	-18.365	-138.4	1.1E
5	B37-1	16-Oct-91	85	3	82	60	532	2.2	177.3	-13	-93	11.9E
6	B37-2	31-Jul-87	190	2.9	92	38.1	533.6	10.1	357	-13.52	-101.4	<0.8E
7	B43-2	21-Apr-83	86	1.5	8.3	0.84	219	7.9	7.5	-13.2	-107	32
8	M1A-3	28-Oct-88	170	2.1	30.2	1.62	158	207.1	128.1	-16.56	-120.3	<0.8E
9	M1B-2	14-Aug-87	27	2.1	35	13.9	254.46	1.9	6.84	-13.12	-99.51	10
10	M2A-3	29-May-86	66	1.47	18.5	4.2	234	20	9.8	-13.62	-104.1	2.5E
11	M2B-2	09-Aug-87	43	1.6	44	9.07	289.2	3.6	6.72	-13.3	-100.5	10
12	M3A-3	07-Jul-88	1680	4.5	491	5.1	53.6	3006	756.7	-17.46	-127	<0.8E
13	M3B-2	29-Jul-87	9.1	1.2	30	5.41	122.9	6.6	18.84	-11.76	-93.11	37
14	M4A-1	02-Dec-83	88	0.88	9.9	4.5	245	28	11.5	-12.9	-102	21
15	M4A-2	06-Dec-83	73	0.71	6.4	2.4	142	45.7	17.3	-13.4	-107	37
16	M4A-3	07-Dec-83	111	1.1	9.8	3	169	64.7	26.3	-13.8	-108	<8.0
17	M4A-4	14-Jul-86	440	2.56	121	3.9	71.5	651.8	325	-18.47	-135.8	<0.8E
18	M5A	12-May-83	292	0.07	19.6	0.33	125	281	149	-18.3	-142	<8.0
19	M5A	16-Sep-83	1200	5.7	1480	11.7	32.2	3980	876	-17.4	-126	<8.0
20	M5B	18-Sep-83	110	2.5	9.9	1.74	187	29.8	52.2	-15.2	-115	19.0E
21	M6-2	07-Aug-86	51	2.2	19.4	3.7	231.9	1.63	11.4	-13.52	-98.4	10.7E
22	M7-72	31-Oct-83	90	3.27	100	10.2	212	207	26	-13.6	-98	<8
23	M7-4	05-Sep-86	1800	7.8	3700	14	14.6	8600	760	-15.54	-112	1.8E
24	M8-3	09-Jun-86	70	1.02	14	1.66	204	21.2	14.2	-14.14	-108.7	7.4E
25	M9-3	18-Jul-88	40	1.23	20	7.7	207	6	5.5	-13.66	-100.6	20E
26	M10-1	11-Nov-88	69	2.1	26.4	3.4	185.545687	35.8	25.3	-14.495	-105.35	9.5E
27	M10-3	15-Apr-86	1010	5.2	1180	10.9	30.4	3020	760	-18.13	-137.3	1.6E
28	M11-2	30-Nov-83	62	1.55	22.1	4.6	236	2.4	8.18	-13.3	-109	7
29	M11-3	21-Jul-88	440	2.8	145	9.9	276.25	589.8	380	-18.54	-140.5	8.8E
30	M12-93	06-Sep-83	81	3.4	15.6	2	246	5.48	6.39	-14.2	-114	<8
31	**M12-159**	**26-Aug-83**	**98**	**0.87**	**6.7**	**0.72**	**255**	**6.71**	**7.2**	**-13.4**	**-105**	**18**
32	M12-171	28-Jul-83	107	0.77	2.1	0.16	230	24	12.9	-13.9	-113	15
33	M13-2	17-Jun-86	810	4.7	185	7.1	32.4	1240	675	-19.65	-148.7	<0.8E
34	M14-1	10-Aug-88	82	2.4	18.3	3.5	229.5	19.5	17.4	-13.76	-103.5	1.3E
35	M14-2	27-Jan-84	134	3.7	20.5	2.4	194	86.8	57.3	-14.5	-112	32
36	M14-4	03-Jun-86	1540	5.6	2600	17.7	18.5	5800	1138	-17.42	-142.2	<0.8E
37	URL1-4	09-Sep-83	13.7	2.43	32.6	7.2	147	11.1	4.7	-12	-93	3
38	URL3-5	02-Dec-83	173	0.8	3.1	0.35	177	96.6	57.7	-13.2	-104	3
39	URL3-6	20-Aug-88	76	2.6	17.5	4.2	200	11.7	27.8	-13.85	-108.7	3.8E
40	URL4-5	23-Jul-86	38	2.27	32	4.9	210.2	0.8	4	-13.5	-102.2	22.7E

	Sample name	Date	Reference water		Approx. zone depth (m)	Mixing p. Brine	Mixing p. Saline	Mixing p. Glacial	Mixing p. Biogen	Mixing p. Precipit.
1			**End-member brine**			**100%**	**0%**	**0%**	**0%**	**0%**
2			**Precipitation**			**0%**	**0%**	**0%**	**0%**	**100%**
3			**Glacial melt-water**			**0%**	**0%**	**100%**	**0%**	**0%**
4	B34-2	28-Jul-88		-4	40	6%	6%	57%	24%	6%
5	B37-1	16-Oct-91		-5	22	3%	3%	4%	87%	3%
6	B37-2	31-Jul-87		-3	45	2%	2%	9%	84%	2%
7	B43-2	21-Apr-83		-3	123	0%	0%	0%	93%	6%
8	M1A-3	28-Oct-88		-7	265	3%	3%	31%	61%	3%
9	M1B-2	14-Aug-87		-3	75	2%	2%	3%	92%	2%
10	M2A-3	29-May-86		-4	310	1%	1%	6%	90%	1%
11	M2B-2	09-Aug-87		-5	150	1%	1%	1%	96%	2%
12	M3A-3	07-Jul-88		-4	375	10%	10%	56%	13%	10%
13	M3B-2	29-Jul-87		-1	120	1%	1%	1%	56%	40%
14	M4A-1	02-Dec-83		-15	180	0%	0%	0%	89%	10%
15	M4A-2	06-Dec-83		-2	215	1%	1%	2%	96%	1%
16	M4A-3	07-Dec-83		-7	260	2%	2%	10%	85%	2%
17	M4A-4	14-Jul-86		-6	310	5%	5%	53%	32%	5%
18	M5A	12-May-83		-3	165	1%	1%	47%	49%	1%
19	M5A	16-Sep-83		-IN8	340	10%	15%	55%	10%	10%
20	M5B	18-Sep-83		-IN9	120	2%	2%	16%	79%	2%
21	M6-2	07-Aug-86		-5	110	2%	2%	2%	93%	2%
22	M7-72	31-Oct-83		-DH	72	3%	3%	6%	85%	3%
23	M7-4	05-Sep-86		-11	390	13%	21%	40%	13%	13%
24	M8-3	09-Jun-86		-7	360	1%	1%	10%	87%	1%
25	M9-3	18-Jul-88		-3	230	1%	1%	3%	93%	1%
26	M10-1	11-Nov-88		-7	50	2%	2%	11%	83%	2%
27	M10-3	15-Apr-86		-2	410	8%	13%	62%	8%	8%
28	M11-2	30-Nov-83		-12	140	1%	1%	6%	91%	1%
29	M11-3	21-Jul-88		-4	290	3%	3%	48%	44%	3%
30	M12-93	06-Sep-83		-DH	93	1%	1%	11%	84%	1%
31	**M12-159**	**26-Aug-83**	**Biogen**	**-18DH**	**159**	**0%**	**0%**	**0%**	**100%**	**0%**
32	M12-171	28-Jul-83		-15DH	171	0%	0%	7%	92%	0%
33	M13-2	17-Jun-86		-5	250	6%	11%	71%	6%	6%
34	M14-1	10-Aug-88		-4	50	2%	2%	7%	87%	2%
35	M14-2	27-Jan-84		-13	105	2%	2%	9%	85%	2%
36	M14-4	03-Jun-86		-4	370	4%	27%	61%	4%	4%
37	URL1-4	09-Sep-83		-24	110	3%	3%	3%	75%	15%
38	URL3-5	02-Dec-83		-1	120	2%	2%	7%	88%	2%
39	URL3-6	20-Aug-88		-9	140	2%	2%	11%	82%	2%
40	URL4-5	23-Jul-86		-10	65	1%	1%	1%	94%	2%

	Sample name	Date	Deviation 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 18O (SMOW)	Deviation 2H (SMOW)	Deviation 3H (TU)
1			**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
2			**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
3			**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
4	B34-2	28-Jul-88	-403	0	-2425	6	-84	-4643	207	2	13	-9
5	B37-1	16-Oct-91	-379	1	-1133	57	302	-2545	130	1	12	-7
6	B37-2	31-Jul-87	-176	1	-817	35	302	-1891	320	1	9	-16
7	B43-2	21-Apr-83	-25	1	-62	0	-19	-132	-1	0	-4	9
8	M1A-3	28-Oct-88	-232	0	-1058	-3	-54	-2057	83	0	10	-13
9	M1B-2	14-Aug-87	-298	0	-724	12	15	-1586	-25	1	6	-8
10	M2A-3	29-May-86	-184	0	-504	2	-7	-1067	-15	1	5	-15
11	M2B-2	09-Aug-87	-157	0	-301	8	43	-714	-12	0	4	-9
12	M3A-3	07-Jul-88	357	-2	-3682	-6	-84	-5734	609	3	18	-11
13	M3B-2	29-Jul-87	-212	0	-504	4	-23	-1112	-3	1	2	-9
14	M4A-1	02-Dec-83	-32	0	-99	4	17	-195	1	0	0	-4
15	M4A-2	06-Dec-83	-131	-1	-352	1	-105	-701	-2	0	-2	19
16	M4A-3	07-Dec-83	-185	-1	-673	0	-66	-1358	-4	1	5	-9
17	M4A-4	14-Jul-86	-225	-1	-1892	-4	-107	-3544	248	1	14	-10
18	M5A	12-May-83	58	-2	-563	-5	-85	-908	120	1	5	-2
19	M5A	16-Sep-83	-562	-1	-2978	-1	-97	-5888	687	2	18	-4
20	M5B	18-Sep-83	-176	1	-659	-1	-44	-1360	22	0	3	3
21	M6-2	07-Aug-86	-237	1	-615	2	-10	-1325	-17	0	6	-8
22	M7-72	31-Oct-83	-382	1	-1145	7	-16	-2403	-22	0	9	-10
23	M7-4	05-Sep-86	-715	-1	-2190	-1	-96	-4746	497	3	14	-13
24	M8-3	09-Jun-86	-145	0	-403	0	-36	-844	-7	0	4	-9
25	M9-3	18-Jul-88	-221	0	-527	6	-36	-1136	-20	0	5	2
26	M10-1	11-Nov-88	-269	0	-798	1	-46	-1684	-10	0	7	-7
27	M10-3	15-Apr-86	-605	-1	-2570	-2	-106	-5466	587	2	15	-8
28	M11-2	30-Nov-83	-149	0	-372	3	-7	-816	-12	1	1	-10
29	M11-3	21-Jul-88	47	0	-964	3	77	-1706	333	0	6	-2
30	M12-93	06-Sep-83	-178	2	-549	0	10	-1168	-20	1	0	-9
31	**M12-159**	**26-Aug-83**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
32	M12-171	28-Jul-83	4	0	-43	-1	-19	-58	4	0	-1	-2
33	M13-2	17-Jun-86	-494	-1	-2652	-6	-114	-5282	533	2	16	-6
34	M14-1	10-Aug-88	-235	1	-728	1	-6	-1539	-15	1	6	-16
35	M14-2	27-Jan-84	-190	2	-752	0	-40	-1527	24	0	-1	15
36	M14-4	03-Jun-86	-1469	-3	-990	-2	-105	-4515	839	3	13	-4
37	URL1-4	09-Sep-83	-445	0	-1203	5	-52	-2581	-42	2	8	-24
38	URL3-5	02-Dec-83	-127	-1	-683	-2	-61	-1335	28	1	5	-14
39	URL3-6	20-Aug-88	-273	1	-845	1	-31	-1788	-8	1	4	-13
40	URL4-5	23-Jul-86	-233	1	-547	3	-32	-1210	-22	0	2	4

	Sample	Date	Measured	Measured	Measured	Measured	Measured	Measured	Measured	Measured	Measured	Measured
	name		Na	K	Ca	Mg	HCO3	Cl	SO4	18O	2H	3H
			(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(SMOW)	(SMOW)	(TU)
41	URL5-4	11-May-82	145	2.76	7.5	1.61	220	84	34	-14.5	-111	<8
42	URL6	12-Jul-83	280	4.33	21.5	3.5	147	336	76	-15.2	-116	92
43	URL7	22-Aug-82	23.4	1.98	26.5	12	208	1.1	7.5	-13.2	-98	33
44	URL8-7	14-Aug-84	81	2	22.2	4.3	219	31	17.2	-14.4	-108	<8
45	URL10-3	09-May-86	22.1	2.01	35.4	10	185	1.46	16.4	-14.11	-109.1	18.3E
46	URL10-6	24-Jun-86	172	2.9	35	3.9	182	155	98.6	-15.95	-118.4	3.5E
47	URL11-3	20-Jul-84	10.6	2.31	49	8.3	181	5.1	22.6	-13.2	-107	51
48	URL11-7	29-Nov-88	72	1.5	25.1	5.5	221.7	4.3	40.2	-13.75	-100.7	23.0E
49	URL12-10	11-Apr-90	735	2.62	156	3.44	51.7	1246	216.8	-17.53	-127.55	<0.8E
50	URL12-11	11-Sep-86	93	3.3	37	3.6	118.6	96	61	-13.28	-103	21.5E
51	URL12-13	22-Jul-86	530	10.2	1070	25	31.9	2454	776	-15.41	-127.7	14.2E
52	URL14	23-Jul-87	1800	4.9	710	8.05	14.5	3389	732	-16.55	-120.9	<0.8E
53	URL15-1	26-May-88	200	5.4	30	3.8	222	190.5	93	-13.55	-104.7	<6.0
54	URL16-4	24-Aug-88	52	3.5	35.3	8.5	184	17.7	36.6	-11.15	-93	20.5E
55	WA1-1	10-Jul-87	9.3	8	40	2.34	118.5	6.9	3.12	-12.03	-99.15	19
56	WA1-2	29-Jun-87	26	4.5	44	9.7	256	1.9	1.7	-11.29	-95.2	11.1E
57	WA1-3	08-Nov-87	84	2.45	35	5.5	321.2	10.8	11.4	-13.81	-104.6	11.1E
58	WA1-5	18-Mar-88	1100	12	1714	44.4	35	3800	1323	-19.04	-139.6	1.3E
59	WB1-1	05-Jun-87	80	4	43	8.3	251.6	56.8	21.3	-12.42	-94.5	17.3E
60	WB1-2	05-Jun-87	260	6	69	10.3	156.7	300	272	-13.47	-104.7	10.8E
61	WB1-4	05-Aug-87	5200	15	725	11.7	16.5	9797	1320	-11.3	-88.85	13.3E
62	WB1-5	06-Oct-87	3100	17	3590	37	14	10780	990	-14.12	-105.3	7.3E
63	**WB1-7**	**30-May-88**	**11000**	**24**	**8410**	**51.1**	**9.9**	**30200**	**1040**	**-12.96**	**-94.35**	**2.1E**
64	WB2-20	12-Mar-91	4360	14.25	10540	34.2	20.1	27900	835	-15.4	-102	<0.8E
65	WD1-110	03-Sep-88	81	1.8	12.3	2.94	241.3	2.8	11.2	-13.82	-106.8	16
66	WD2-72	01-Sep-88	59	2.6	28	5.5	255	1.6	11.7	-13.45	-103.4	10.2E
67	WD3-895	14-Sep-88	1900	7.9	4300	40	26.2	11390	492	-15.62	-113.15	5.2E
68	WG2-2	15-May-87	70	2.6	13.4	2.71	218.5	3.3	7.4	-13.04	-100.3	9.0E
69	WN1-8	24-May-87	1400	8	1150	53.3	73	3480	770	-16.18	-117.4	2.6E
70	WN3	20-Aug-79	160	3.3	25.4	11.1	328	119	82	-16.2	-122	<8
71	WN4-6	08-May-87	1400	9	1370	60.8	60.8	3880	890	-16.54	-120.6	59
72	WN4-13	11-Dec-89	4890	10.5	2687	25.5	15	11091	1393.1	-15.95	-116.5	<0.8E
73	WN8	26-Aug-88	1060	5.3	740	39.8	85.2	2581	630	-16.78	-124.5	1.6E
74	WN10-3	09-Dec-88	770	5.6	289	27	71	1350	700	-17.87	-132.4	<0.8E
75	WN10-4	26-Mar-87	1330	8.7	910	66	27	2909	1400	-18.14	-131.3	2.3E
76	WN11-17	09-Dec-86	6800	19.1	4930	26.7	19.6	18944	1105	-14.12	-109.1	3.0E

	Sample name	Date	Reference water		Approx. zone depth (m)	Mixing p. Brine	Mixing p. Saline	Mixing p. Glacial	Mixing p. Biogen	Mixing p. Precipit.
41	URL5-4	11-May-82		-43	100	2%	2%	12%	82%	2%
42	URL6	12-Jul-83		-25	270	1%	1%	1%	94%	2%
43	URL7	22-Aug-82		-24	60	1%	1%	1%	81%	15%
44	URL8-7	14-Aug-84		-6	230	2%	2%	11%	84%	2%
45	URL10-3	09-May-86		-2	80	2%	2%	11%	83%	2%
46	URL10-6	24-Jun-86		-7	250	3%	3%	26%	66%	3%
47	URL11-3	20-Jul-84		-1	45	1%	1%	1%	85%	12%
48	URL11-7	29-Nov-88		-7	135	1%	1%	2%	95%	1%
49	URL12-10	11-Apr-90		-19	390	6%	6%	45%	38%	6%
50	URL12-11	11-Sep-86		-13	430	3%	3%	6%	84%	3%
51	URL12-13	22-Jul-86		-21	605	12%	15%	50%	12%	12%
52	URL14	23-Jul-87		-8	280	12%	12%	52%	13%	12%
53	URL15-1	26-May-88		-4	125	4%	4%	9%	80%	4%
54	URL16-4	24-Aug-88		-1	85	2%	2%	2%	52%	41%
55	WA1-1	10-Jul-87		-3	150	5%	5%	5%	63%	22%
56	WA1-2	29-Jun-87		-8	240	2%	2%	2%	57%	36%
57	WA1-3	08-Nov-87		-8	320	1%	1%	2%	96%	1%
58	WA1-5	18-Mar-88		-7	630	-	-	-	-	-
59	WB1-1	05-Jun-87		-5	130	2%	2%	2%	66%	28%
60	WB1-2	05-Jun-87		-6	230	6%	6%	15%	67%	6%
61	WB1-4	05-Aug-87		-SW10	540	15%	37%	19%	15%	15%
62	WB1-5	06-Oct-87		-21	630	9%	45%	30%	9%	9%
63	**WB1-7**	**30-May-88**	**Saline**	**-7**	**1000**	**0%**	**100%**	**0%**	**0%**	**0%**
64	WB2-20	12-Mar-91		-12	725	8%	63%	15%	8%	8%
65	WD1-110	03-Sep-88		-2	100	1%	1%	5%	93%	1%
66	WD2-72	01-Sep-88		-5	65	1%	1%	3%	92%	1%
67	WD3-895	14-Sep-88		-10	810	12%	26%	38%	12%	12%
68	WG2-2	15-May-87		-8	130	2%	2%	2%	91%	3%
69	WN1-8	24-May-87		-17	380	8%	24%	51%	8%	8%
70	WN3	20-Aug-79		-90	90	1%	1%	23%	73%	1%
71	WN4-6	08-May-87		-8	370	10%	22%	47%	10%	10%
72	WN4-13	11-Dec-89		-20	650	3%	49%	42%	3%	3%
73	WN8	26-Aug-88		-T4	315	10%	13%	56%	10%	10%
74	WN10-3	09-Dec-88		-4	245	9%	12%	62%	9%	9%
75	WN10-4	26-Mar-87		-3	320	-	-	-	-	-
76	WN11-17	09-Dec-86		-15	1000	4%	66%	21%	4%	4%

	Sample	**Date**	**Deviation**	**Deviation**	**Deviation**	**Deviation**	**Deviation**	**Deviation**	**Deviation**	**Deviation**	**Deviation**	**Deviation**
	name		**Na**	**K**	**Ca**	**Mg**	**HCO3**	**Cl**	**SO4**	**18O**	**2H**	**3H**
			(mg/l)	**(mg/l)**	**(mg/l)**	**(mg/l)**	**(mg/l)**	**(mg/l)**	**(mg/l)**	**(SMOW)**	**(SMOW)**	**(TU)**
41	URL5-4	11-May-82	-155	1	-694	-1	-13	-1378	3	0	4	-8
42	URL6	12-Jul-83	18	3	-528	2	-96	-812	51	-2	-11	73
43	URL7	22-Aug-82	-240	1	-569	10	-1	-1245	-18	0	3	5
44	URL8-7	14-Aug-84	-197	0	-604	2	-17	-1272	-11	0	5	-9
45	URL10-3	09-May-86	-306	0	-754	7	-48	-1647	-17	1	4	1
46	URL10-6	24-Jun-86	-240	1	-1072	-1	-33	-2151	53	1	8	-11
47	URL11-3	20-Jul-84	-190	1	-329	7	-38	-784	4	0	-5	25
48	URL11-7	29-Nov-88	-174	0	-470	4	-23	-1030	17	0	4	5
49	URL12-10	11-Apr-90	-6	-1	-2085	-4	-129	-3434	133	1	13	-11
50	URL12-11	11-Sep-86	-402	1	-1287	1	-108	-2679	10	1	4	3
51	URL12-13	22-Jul-86	-1285	3	-3852	12	-93	-8255	580	4	10	1
52	URL14	23-Jul-87	315	-2	-3984	-3	-116	-6451	567	3	18	-13
53	URL15-1	26-May-88	-337	3	-1438	0	0	-2886	37	1	4	-12
54	URL16-4	24-Aug-88	-300	2	-930	7	46	-2008	0	2	2	-26
55	WA1-1	10-Jul-87	-668	5	-1933	-1	-53	-4136	-68	2	0	-12
56	WA1-2	29-Jun-87	-298	3	-815	8	105	-1799	-32	2	1	-32
57	WA1-3	08-Nov-87	-74	1	-175	4	72	-423	-3	0	2	-7
58	WA1-5	18-Mar-88	-	-	-	-	-	-	-	-	-	-
59	WB1-1	05-Jun-87	-246	2	-796	7	78	-1703	-12	1	4	-19
60	WB1-2	05-Jun-87	-547	2	-2300	5	-44	-4670	186	2	7	-7
61	WB1-4	05-Aug-87	931	2	-6946	-9	-64	-9100	892	4	14	-3
62	WB1-5	06-Oct-87	-1951	4	-2863	11	-68	-7291	496	3	13	-3
63	**WB1-7**	**30-May-88**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
64	WB2-20	12-Mar-91	-2643	-3	2922	1	-34	4991	160	0	2	-9
65	WD1-110	03-Sep-88	-110	1	-313	1	-4	-671	-7	0	2	-1
66	WD2-72	01-Sep-88	-211	1	-550	4	13	-1206	-15	0	3	-8
67	WD3-895	14-Sep-88	-1162	-2	-1623	23	-79	-2830	180	2	12	-8
68	WG2-2	15-May-87	-242	1	-704	1	-18	-1498	-23	1	4	-10
69	WN1-8	24-May-87	-1370	-1	-3472	36	-45	-8169	489	3	24	-7
70	WN3	20-Aug-79	-71	2	-484	8	100	-930	57	0	4	-6
71	WN4-6	08-May-87	-1180	0	-3734	45	-55	-8273	624	2	15	47
72	WN4-13	11-Dec-89	-602	-3	-2364	-4	-74	-5341	864	2	20	-3
73	WN8	26-Aug-88	-589	-2	-3600	27	-46	-6925	451	3	21	-10
74	WN10-3	09-Dec-88	-720	-1	-3455	14	-66	-6940	538	3	20	-9
75	WN10-4	26-Mar-87	-	-	-	-	-	-	-	-	-	-
76	WN11-17	09-Dec-86	-496	2	-1941	-9	-38	-3179	406	2	4	-3

	Sample name	**Date**	**Measured Na (mg/l)**	**Measured K (mg/l)**	**Measured Ca (mg/l)**	**Measured Mg (mg/l)**	**Measured HCO3 (mg/l)**	**Measured Cl (mg/l)**	**Measured SO4 (mg/l)**	**Measured 18O (SMOW)**	**Measured 2H (SMOW)**	**Measured 3H (TU)**
			Boundarie conditions									
	ul		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
	ll, M5A	*16-Sep-83*	*1200*	*5.7*	*1480*	*11.7*	*32.2*	*3980*	*876*	*-17.4*	*-126*	*8*
	ur, M12-159	*26-Aug-83*	*98*	*0.87*	*6.7*	*0.72*	*255*	*6.71*	*7.2*	*-13.4*	*-105*	*18*
	lh, URL12-13	*22-Jul-86*	*530*	*10.2*	*1070*	*25*	*31.9*	*2454*	*776*	*-15.41*	*-127.7*	*14.2*
	top1		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
	top2		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
	top3		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
	top4		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
	top5		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
	top6		*0.29*	*0.31*	*0.55*	*0.085*	*1.85*	*0.44*	*1.09*	*-11.3*	*-80*	*90*
			Bold marks reference water									
			Grey shaded cells are samples included in Kriging/Surfer mod.									
			Italics marks boundaries									
			E indicates tritium analysis of groundwater enriched by electrolysis									

	Sample name	Date	Reference water		Approx. zone depth (m)	Mixing p. Brine	Mixing p. Saline	Mixing p. Glacial	Mixing p. Biogen	Mixing p. Precipit.
	ul		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*
	ll, M5A	*16-Sep-83*		*-IN8*	*340*	*10%*	*15%*	*55%*	*10%*	*10%*
	ur, M12-159	*26-Aug-83*	*Biogen*	*-18DH*	*159*	*0%*	*0%*	*0%*	*100%*	*0%*
	lh, URL12-13	*22-Jul-86*		*-21*	*605*	*12%*	*15%*	*50%*	*12%*	*12%*
	top1		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*
	top2		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*
	top3		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*
	top4		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*
	top5		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*
	top6		*Precipitation*			*0%*	*0%*	*0%*	*0%*	*100%*

	Sample	Date	Deviation	Deviation	Deviation	Deviation	Deviation	Deviation	Deviation	Deviation	Deviation	Deviation
	name		Na	K	Ca	Mg	HCO3	Cl	SO4	18O	2H	3H
			(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(mg/l)	(SMOW)	(SMOW)	(TU)
	ul		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	ll, M5A	*16-Sep-83*	*-562*	*-1*	*-2978*	*-1*	*-97*	*-5888*	*687*	*2*	*18*	*-4*
	ur, M12-159	*26-Aug-83*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	lh, URL12-13	*22-Jul-86*	*-1285*	*3*	*-3852*	*12*	*-93*	*-8255*	*580*	*4*	*10*	*1*
	top1		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	top2		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	top3		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	top4		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	top5		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
	top6		*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*