

**An approach to quality classification
of deep groundwaters in Sweden
and Finland**

Marcus Laaksoharju¹, John Smellie²,
Paula Ruotsalainen³, Margit Snellman⁴

1 GeoPoint AB, Stockholm, Sweden

2 Conterra AB, Uppsala, Sweden

3 Fintact Ky, Helsinki, Finland

4 Imatran Voima Oy, Vantaa, Finland

November 1993

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- 1 GeoPoint AB, Stockholm, Sweden
- 2 Conterra AB, Uppsala, Sweden
- 3 Fintact Ky, Helsinki, Finland
- 4 Imatran Voima Oy, Vantaa, Finland

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

Information on SKB technical reports from 1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40), 1990 (TR 90-46), 1991 (TR 91-64) and 1992 (TR 92-46) is available through SKB.

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Marcus Laaksoharju
GeoPoint AB
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John Smellie
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Uppsala

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Fintact Ky
Helsinki

Margit Snellman
Imatran Voima Oy
Vantaa

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This report is also published in the YJT Technical Report series of Nuclear Waste Commission of Finnish Power Companies

ABSTRACT

The quality and representativeness of groundwaters sampled in the Swedish SKB and in the Finnish TVO nuclear waste disposal site investigations have been evaluated. By definition a high quality sample is considered to be the one which best reflects the undisturbed hydrological and geochemical in situ conditions for the sampled section. Manual (expert judgement), statistical multivariate, mixing models and quality scoring system have been used to classify the waters regarding representativity. The constructed scoring system is best suited for quality classification, although the expert judgement is always needed as a complement. The observations are scored on a continuous scale based on the response of selected quality indicating parameters. Less representative samples are not rejected but given a value indicating the confidence of the observation. Finnish data obtained 45% of the possible scores compared to 55% for the Swedish data. The quality is generally 10% higher in the Swedish samples compared to the Finnish samples. The difference in sampling procedure is the probable reason for this.

SAMMANFATTNING

Kvaliten och representativiteten för de grundvattenprover som samlats inom svenska SKB:s och finska TVO:s undersökningar för förvaring av kärnavfall har utvärderats. Definitionsmässigt anses prov av hög kvalitet vara ett som bäst speglar ostörda hydrologiska och geokemiska in situ förhållanden för den provtagna (borrhåls)sektionen. För att klassificera vattenproverna med avseende på representativitet har manuella metoder (expertbedömning), statistiska multivariat, blandningsmodeller och poängsättningssystem prövats. Poängsättningssystem är bäst lämpat för kvalitetsklassificering även om expertbedömning alltid behövs som komplement. Observationerna poängsätts på en fortlöpande skala, baserad på utslaget av utvalda kvalitetsindikerande parametrar. Mindre representativa prover förkastas inte men de ges ett värde som indikerar observationens tillförlitlighet. Finska data erhöll 45 % av möjliga poäng jämfört med 55% för svenska data. Kvaliten är generellt 10% högre i de svenska proverna jämfört med de finska. Anledningen till detta är troligtvis skillnaden i insamlingsförfarandet.

SUMMARY

In Sweden and Finland high quality groundwater samples are required in the site characterisation programmes relating to safe disposal of spent nuclear fuel. SKB (Swedish Nuclear Fuel and Waste Management Co.) and TVO (Teollisuuden Voima Oy, Finland) initiated a co-operative task to critically evaluate the quality of the earlier sampling programmes and to further develop the understanding of quality or representativeness of the groundwater samples. The major aim in this report has been, therefore, to make an attempt to classify groundwaters from site investigations in Sweden and Finland based on quality. Different classification systems have been tested and developed. These can be divided in two main groups; manual methods and computer-based mathematical methods. Manual, statistical, mixing ratio and scoring systems have all been used to illustrate the difficulty in judging groundwater quality.

Manual systems sort observations into useful and less useful categories, and are usually based on quality-indicating parameters and calculations combined with experience of groundwater systems and logical judgement. A certain amount of subjectivity is sometimes necessary to judge how important certain variables are, and to predict their consequences. The advantage is that qualitative information which may be difficult to express mathematically can be incorporated. The inter-relationships between quantitative and qualitative data often prove to be decisive factors in groundwater quality evaluation. In addition, the manual treatment is flexible, site- or borehole-specific, and is also an essential part of the initial sorting and interpretation stage of the data. Disadvantages may include the difficulty of reproducibility since some of the criteria cannot be quantitatively described, thus introducing a degree of subjectivity. Also, different people may tend to emphasise different parameters of importance. Furthermore, the manual procedure may sometimes be too strict, for example, observations of lower quality are often not considered for further evaluation.

The mathematical models score observations on a continuous scale based on the response of selected quality indicating parameters. The less representative samples are not rejected but given a value indicating the confidence of the observation. Loss of information, effort and investment is hence minimised. Even though the selected models and assumptions are based on experience and logical judgement, which maybe somewhat subjective, they are strictly formulated so that reproducibility is reliable. The steps and models are well documented, which contrasts with the manual approach. The systems also handle many variables and a large amount of data with the same effort as using few observations. Furthermore, the models may be later modified and changed based on new data or site specific needs. The main disadvantage is that the mathematical models tend to simultaneously oversimplify the system leading to a loss of sensitivity. Incomplete data sets for some variables may also lend bias to the results. There is also the danger that mathematical systems might become "blackboxes" which automatically process results. The system is no better than the quality of the input data, the logical judgement used to formulate the parameters/criteria of importance and, ultimately, belief in the model.

The general absence of consistent groundwater sampling policy and the use of different, sampling methodologies and techniques, is reflected in most of the classifications presented in this report. Some credence has been found within individual site-specific areas (i.e. the manual system), but there has been a failure to adequately compare groundwater quality data between individual sites (since each site appears to be hydrogeologically unique) and also between the SKB and TVO hydrogeochemical programmes. The respective sites are geologically and hydraulically too complex, and the groundwater quality-influencing factors too numerous, to describe, quantify and compare. Of the methods used, only the quality scoring system has managed to circumvent some of these problems by identifying and comparing mathematically chosen variables irrespective of the methodology or equipment used to measure them. According to this method the quality is generally 10% higher in the Swedish samples compared to the Finnish samples. However, only general comparisons can be made, any detailed interpretation of the data must rely on expert knowledge and experience. A method of general quality evaluation to produce a suitable hydrogeochemical database for Sweden and Finland has been derived.

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1 INTRODUCTION AND AIM

Groundwater hydrogeochemical data often comprise a large number of variables, all of which contribute a particular piece of information. The history, reactions, mixing situations and the flow paths of the groundwater may be coded in these variables. In order to make best use of these variables the quality of the field and laboratory data must be ensured as the understanding of natural groundwater systems is no better than the data on which they are based.

In Sweden and Finland high quality groundwater samples are needed in the site characterisation programmes related to the disposal of spent nuclear fuel. SKB (Swedish Nuclear Fuel and Waste Management Co.) and TVO (Teollisuuden Voima Oy, Finland) therefore initiated a co-operative task to develop the understanding of quality or representativeness of groundwater samples. The major aim in this report has been to make an attempt to classify groundwaters from site investigations in Sweden and Finland based on quality. Different methods have been tested and developed such that representative chemical compositions can be identified for classification and modelling purposes. In this report by definition *a high quality sample is considered that which best reflects the undisturbed hydrological and geochemical in situ conditions for the sampled section*. A low quality and hence unrepresentative sample reflects in situ, on-line, on-site or off-site errors such as excessively high and low extraction pump-rates, contamination from borehole activities, complex hydrological situations, contamination from tubes of varying compositions, air contamination, losses or uptake of CO₂, long storage times prior to analyses, analytical errors etc. The quality may also be influenced by the rationale in locating the borehole and selecting of the sampling points. Some errors are easily avoidable, others difficult or impossible. Furthermore, chemical responses to these influences are sometimes apparent, but not always.

To consider which activities can disturb or misrepresent the quality of the groundwater chemistry is essential when trying to evaluate the hydrogeochemical evolution of the site under investigation. For example, geochemical equilibrium models are used to understand and detail those water-rock interactions which contribute to the overall chemistry of the groundwaters, and the success of these modelling exercises very much depends on the reliability of the input data. Geosphere transport models, used to study the potential release and transfer of trace elements (e.g. radionuclides) from a deep-seated waste repository to the biosphere, require realistic conceptual models and input data from geological, hydrogeological and hydrochemical sources. Presently such transport models are used to describe scenarios which form the basis of repository performance safety assessment relating to the final disposal of nuclear waste. Usually scenarios are assumed whereupon the retardation of the radionuclides at the engineered barriers and within the surrounding geosphere is often underestimated. Moreover, some of the more conservative assumptions relating to performance assessment are based on inadequate or qualitative groundwater data. When aiming at the optimisation of the repository system a more realistic modelling approach using quantitative site-specific groundwater analytical data of high quality is therefore required.

Programmes of groundwater sampling should be based upon a reliable conceptual model of the groundwater flow system. Even so, the groundwater sampling and monitoring

programme can still be fraught with hazards which can easily influence the quality of the results. To exemplify the difficulty in getting obtaining useful parameter values from field measurements, the calculated and measured pH and Eh values in situ, on-site and off-site are shown in Figure 1. In this particular case the measured off-site pH is closer to the in situ calculated value than the on-line value. The off-site value therefore reflects the in-situ condition better than the on-line value, i.e. the off-site pH is of a higher quality and more representative. The off-site Eh measurement on the other hand is erroneous and the on-line value should thus be selected. In this case the on-line value changes are dependent on the pump-rate; a high pump-rate is favourable since long decompression times (up to 17 h) are avoided prior to analyses. However, on the other hand, an obvious disadvantage is the risk of changing the overall chemistry downhole due to excessive withdrawal of foreign water types at high pump-rates as shown by Smellie (1983) and Laaksoharju et al. (1993). Downhole in situ measurements of Eh and pH are to be preferred (Wikberg, 1987).

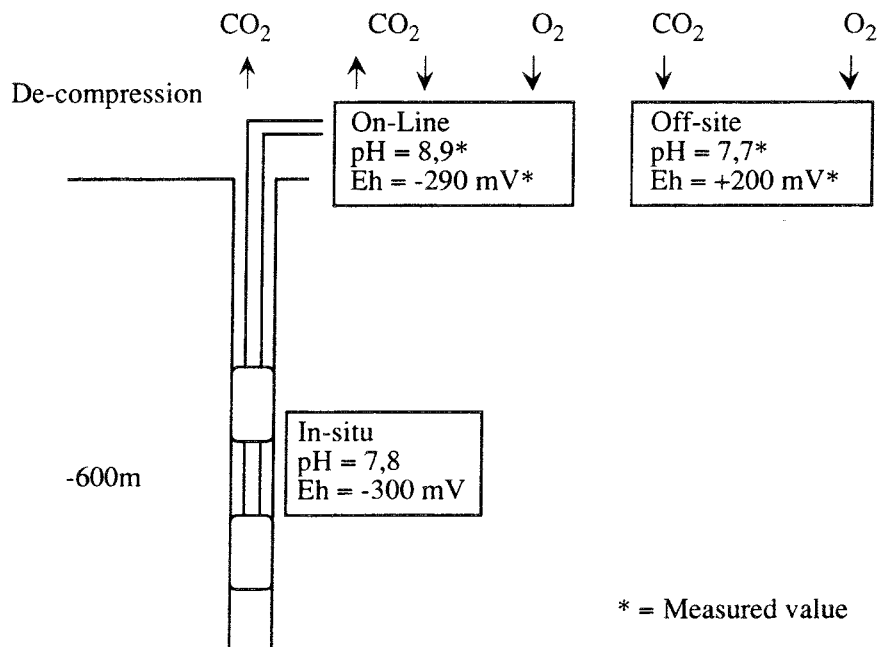


Figure 1. The measured and calculated pH and Eh values from a typical deep groundwater system (data from Olkiluoto KR1: 613 - 618 m (Pitkänen et al., 1992; Laaksoharju et al., 1993)). The values are constantly changing, depending on decompression, loss or uptake of CO₂ and O₂. The off-site pH and on-line Eh values are closer to the in-situ values in this particular case.

From the outset of this report it was obvious that to compare existing groundwater data within any one site area, far less between Sweden and Finland, was a major if not an impossible task. The work required in many cases the testing and development of new methods. The data from the site investigation programmes were chosen after first reviewing and classifying available Swedish and Finnish groundwater data (Lampén et al., 1992).

Site-specific investigations in Sweden have been carried out by SKB during the last 16 years. This has resulted in the development and testing of increasingly sophisticated drilling, sampling and analytical techniques (Almén et al., 1986; Almén and Zellman, 1991). Today, this accumulated experience can provide sets of reliable groundwater data collected under stringently controlled conditions. However, direct comparison of data from each of the studied areas is only possible if similar sampling and analytical protocols have been implemented. This, however, has not been the case, as more refined sampling and analytical protocols have been implemented during this 16 year period, resulting in a wide disparity of groundwater quality. Different methods give different results making comparisons difficult.

The Finnish site investigation programme carried out by TVO started in 1984. These studies have resulted in development of field instrumentation and tests which have presently evolved to a novel downhole technique combining in situ measurement of groundwater flow and sampling (Öhberg, 1991; Rouhiainen et al., 1992). The main body of data is from preliminary site investigations in five areas during 1987 - 1992. Some earlier data collected by IVO (Imatran Voima Oy) have been included from studies at Hästholmen, Loviisa. The TVO groundwater hydrogeochemical programme has concentrated on obtaining a more qualitative description of groundwater types prior to their site-specific studies which are scheduled to commence in 1993. The Finnish database contains all the measured and analysed raw values without any pre-quality control as is the case for the Swedish database. The Finnish data also include groundwater data from hydrotests performed using different sampling and analytical techniques. These database differences, plus the fact that the Swedish advanced monitoring techniques combine in-situ Eh and pH measurements with on-site analyses, means that there are different levels of groundwater and analytical quality from the onset.

Given these inherent difficulties, this report describes different approaches to judge the quality and representiveness of groundwaters sampled within the Swedish and Finnish radioactive waste management programmes (Fig. 2). Manual methods, based on experience and intimate knowledge of the sites, are compared with mathematical and statistical methods, considered to be more objective, to try and establish a general protocol that could provide a qualitative and reliable Swedish/Finnish groundwater database (present and future) for use in repository performance assessments.

Essentially, the goal is to establish a simple scoring and ranking system enabling the reliability of data from the different sites to be compared. A ranking system can also be used to weight information so that even low quality data can be used and compared in the right perspective with high quality data. Two main categories have evolved; risk and response judgement systems. The former is mainly based on the presence or absence of important chemical or hydrological factors which may have affected the water quality. The other system searches for a response indication in the chemistry from the above factors. The systems may also be combinations of the two categories. Manual, statistical, mixing ratio and scoring systems have all been used to illustrate the difficulty in judging groundwater quality.

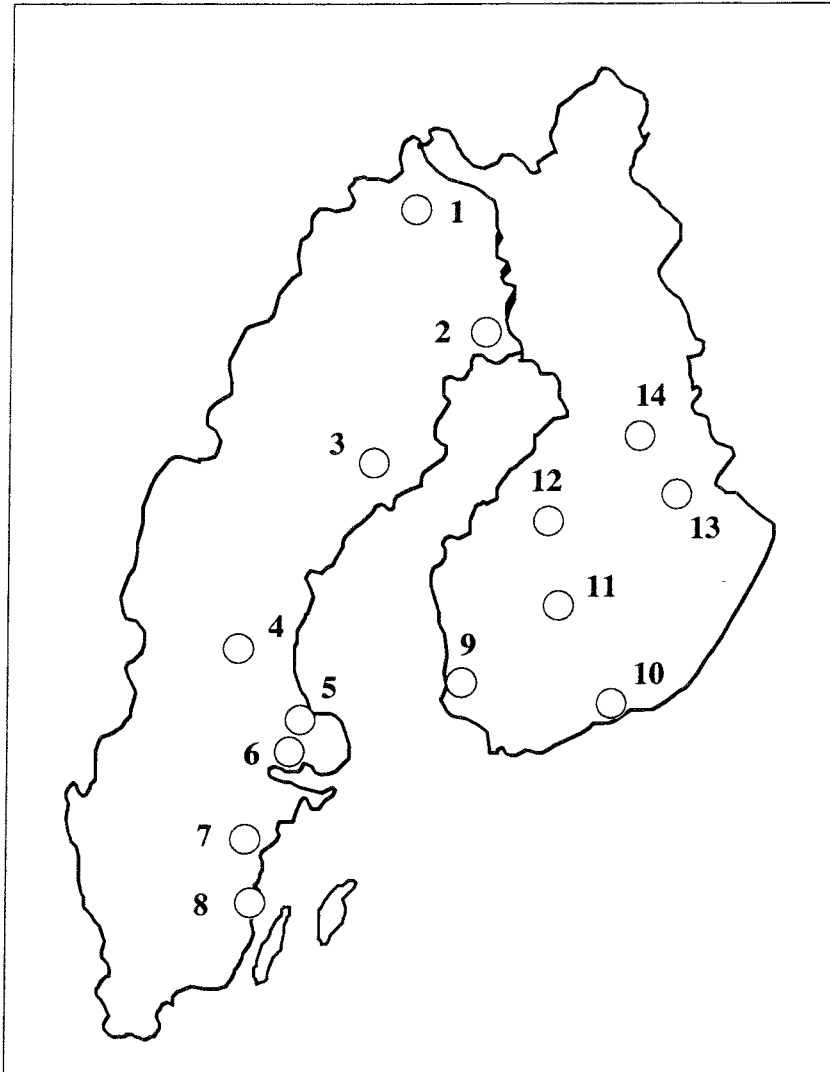


Figure 2. Study sites where groundwater sampling has been performed (Taavinunnanen 1, Kamlunge 2, Gideå 3, Svartboberget 4, Finnsjön 5, Fjällveden 6, Kråkemåla 7, Äspö + Ävrö + Laxemar 8, Olkiluoto 9, Hästholmen 10, Kivetty 11, Syyry 12, Romuvaara 13 and Veitsivaara 14).

2 HISTORICAL BACKGROUND TO QUALITY THINKING

2.1 Introduction

To date within the SKB and TVO site characterisation programmes groundwater quality has been mainly addressed by the manual method. In some cases geochemical equilibrium modelling has been used to correct field data and model the in situ conditions. This essentially means that a synthesis of water quality is based on establishing and understanding the interplay between the many variables which can influence the quality of a sampled groundwater. This is achieved by being familiar with the analytical data and systematically approaching, for example, each borehole and borehole section etc., in order to address the variables which can contribute to (and also identify) all the potential sources which can influence the quality of the groundwater. A certain amount of subjectivity is sometimes necessary to judge how important certain variables are, and to predict their consequences. However, for the geochemist closely linked with the site investigations, this should not pose a major problem as he or she should be aware of, and probably have helped to plan, the programme of investigations with all the accompanying pitfalls and difficulties.

During the period 1976 to 1986, SKB performed surface and borehole investigations of 14 site-specific study areas for the purpose of assessing their suitability as a final repository for high-level spent nuclear fuel. Additional sites include Stripa and, more recently Äspö, which is presently being excavated to house the Hard Rock Laboratory. Groundwater quality evaluations from these earlier sites are discussed below.

2.2 Method

Table 1 lists the parameters used in evaluating the in situ groundwater quality from most of the above-mentioned site areas (Groups I - IV). Sternö, Finnsjön I and Kråkemåla were not assessed due to a lack of quantitative data, and Stripa falls outside the framework of the site-specific study areas.

Using the chemical "Groundwater parameters", the general background chemistry of the site was first thoroughly established by traditional means. For example, concentration/depth plots or piper diagrams generally classified the major groundwater types and further revealed the overall chemical evolution trends with increasing depth (e.g. changes in salinity, redox, pH etc.). Thus, the major chemical groups were recognised and *anomalously high and low values* identified from the analytical data. Then, by systematically applying hydrological and geological considerations ("Hydraulic parameters") coupled with potential sources of contamination ("Borehole activity parameters") it was possible to differentiate between those groundwaters which were reasonably hydrologically representative for the depth sampled, from those where waters from different sources have been introduced from higher or lower bedrock levels. Contamination usually corresponded to the anomalous values identified from the analytical data. This approach is generally simple and straight forward, being based on established concepts of known groundwater evolutionary trends which are then coupled to those measured borehole hydraulic and borehole activity parameters which can influence the groundwater chemistry. Provided that similar chemical

and hydraulic data are available for each sampled location, the procedure can be repeated and compared with reasonable certainty.

One of the most useful exercises carried out was the calculation of the water budget for each sampled borehole section; the description below is taken from Smellie et al. (1987). Calculation of the water budget requires input regarding the amount of:

- borehole drilling water introduced into the borehole section under pressure
- water removed from the borehole during gas-lift pumping
- water introduced into the borehole section during hydraulic injection tests
- water removed from the borehole section during sampling
- water entering or leaving the borehole section during open-hole conditions
- drilling debris introduced into the borehole section under drilling pressure

Boreholes drilled in crystalline rock inevitably influence the groundwater conditions. Furthermore, the actual drilling of the borehole, followed by gas-lift pumping and hydraulic testing, influence both the hydraulic and chemical conditions of the groundwater. The two major sources of influence found are those of drilling and the open-hole effect.

Table 1. Parameters* considered in the manual evaluation and classification of the groundwater quality.

Parameters	Group I	Group II	Group III	Group IV
Groundwater parameters				
pH and alkalinity	x	x	x	x
Na, Ca and Cl contents	x	x	x	x
Redox potential (Eh)	x	x	x	x
Redox-sensitive elements	x	x	x	x
Uranium geochemistry	x	x	x	x
² H, ³ H, ¹⁸ O isotopes	x	x	x	x
²³⁴ U/ ²³⁸ U isotopic ratios	x	x	x	x
Geochemical modelling		x		x
Borehole activity parameters				
Drilling	x	x	x	x
Gas-lift pumping	x	x	x	x
Drilling debris	x	x		
Pump tests				x
Open-hole effects	x	x	x	
Geophysical measurements		x	x	x
Hydraulic injection tests	x	x	x	x
Water sampling	x	x	x	x
Hydraulic parameters				
Hydraulic conductivity	x	x	x	x
Hydraulic head	x	x	x	
Water budget	x	x		
Group I : Svartboberget, Gideå, Fjällveden, Kamlunge, Taavinunnenen Group II : Klipperås Group III : Finnsjön II Group IV : Äspö				
*Note: The number and quality of parameters measured/calculated varies from area to area				

Based on values of drilling rate, drilling water pressure and flow-rate, and the hydraulic conductivity of the borehole, a very rough estimate can be made on the amount of water injected into the bedrock during drilling. It has been calculated, depending on the amount and frequency of fracturing in the bedrock, that more than 100 m³ of flushing water may be lost into the bedrock during drilling. During gas-lift pumping, only a small part of the drilling water is flushed out; consequently most of it remains in the bedrock. Furthermore, the long-term influence of open-hole effects can result in several hundreds of m³ of water per year circulating in the borehole.

During hydraulic testing additional water is injected into the bedrock, although this amount is very small compared to the amount introduced during drilling. Finally groundwater sampling takes place, during which time a somewhat smaller volume of water is removed from the borehole.

In conclusion, some residual contaminating water may still remain in the isolated borehole section under investigation following borehole activities. The extent of contamination is determined largely by the hydraulic character of the intercepted bedrock. Unfortunately, because of the various potential origins to this residual water, the absence of any added tracer (i.e. drilling/injection water) does not necessarily mean an absence of contamination. For example, the existence of misplaced formation water resulting from open-hole effects may only be determined by major chemistry and isotopic signatures.

Figure 3, representing two investigated horizons from the Fjällveden study site (Smellie et al., 1985), presents the calculated amount of water entering and leaving the bedrock enclosing the total length of boreholes Fj2 and Fj4 (disregarding the open-hole effect). The figure also shows the water budget estimations from one of the sampled levels in Fj2 (123 - 126 m borehole length). In this case the long-term importance of the open-hole effect is clearly illustrated, and underlines the fact that analysing for drilling water (e.g. by uranium) will not always result in establishing the presence or absence of borehole contamination.

It should also be noted that the reliability of the water budget calculations is very much dependent on the accuracy and precision of the hydraulic measurements, particularly the use of small straddle lengths to isolate only those conductive sections actually providing the groundwater. This is not an easy task, and it requires close integration of downhole geology, geophysics and hydrogeology.

The influence of drilling debris was addressed by Smellie and Wikberg (1991) from studies of the Finnsjön study site. It is highly plausible that the introduction of such debris during drilling can help seal small-scale hydraulic fractures, thus restricting access to the borehole section to be sampled. In addition, the presence of very fine debris particles in the groundwater can influence studies of colloids (artefacts?), and affect the content of uranium (and Fe if present in sufficiently small quantities) ionic complexes, which may become preferentially bound to these particles and subsequently removed on filtration. Earlier reported studies at Finnsjön (Ahlbom et al. 1986) showed that even after flushing one of the holes twice, only an estimated 5 kg of rock debris were recovered from a calculated total of 1000 kg for a hole 376 m long in crystalline rock with a diameter of 56 mm. Later studies

(Smellie and Wikberg, 1991) showed that the amount of rock debris recovered during drilling decreased markedly with depth from 86.5% down to 85 m and to 41.4% down to 459 m. In this case a total of 8400 kg of debris is calculated to have been forced into the fracture systems intercepted by the borehole, especially at increased depth.

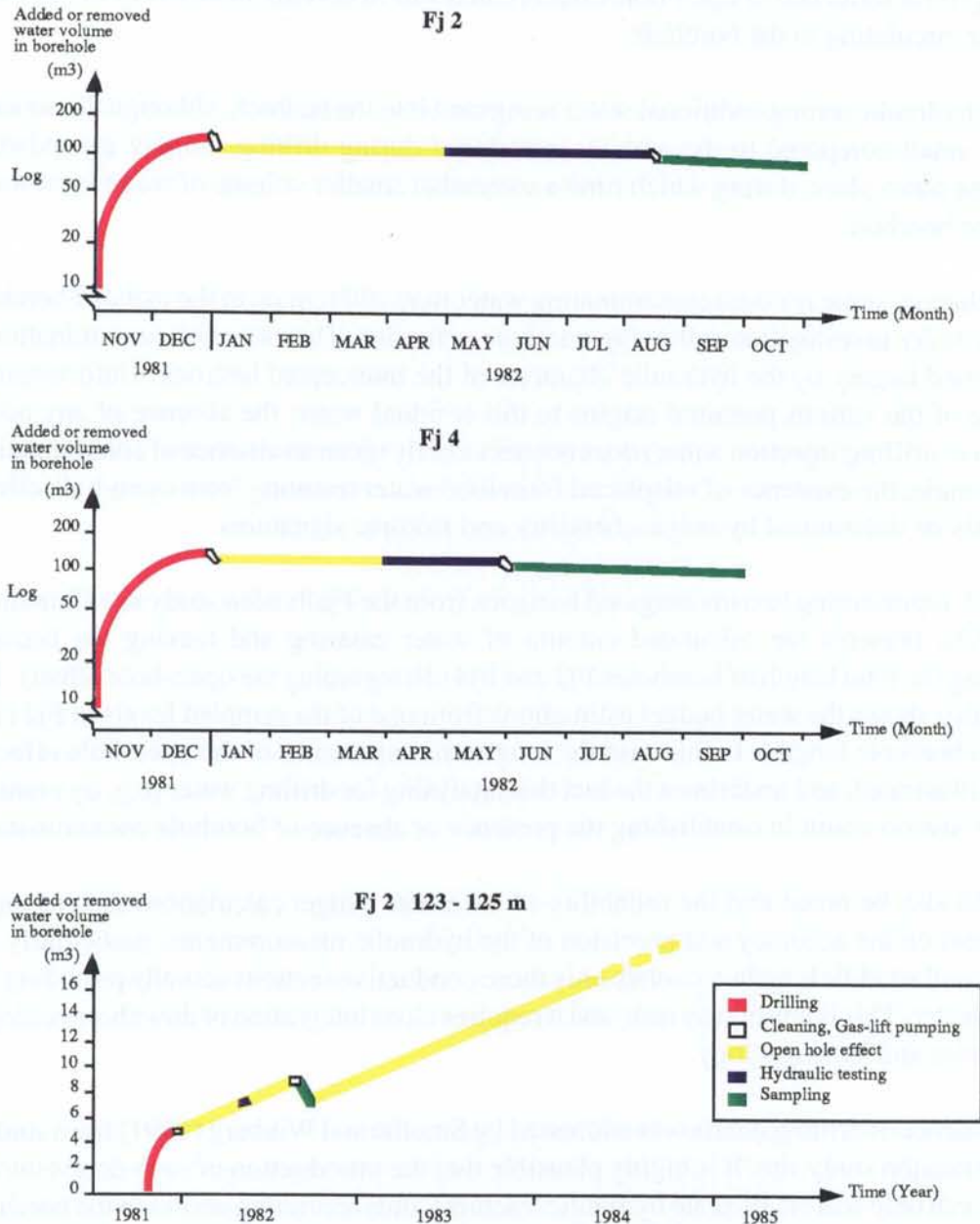


Figure 3. Estimated water budget (i.e. water volumes introduced and extracted) during different activities for boreholes Fj2 and Fj4 disregarding the open-hole effect. The bottom diagram illustrates the water budget for section 123 - 126 m within borehole Fj2 (modified after Smellie et al., 1987).

The manual evaluation of groundwater quality, therefore, has been carried out by a sequence of logical steps which considered each parameter in turn (Table 1), evaluating its influence, if any, and then integrating the result to other parameters that would also be expected to be influenced. For example, drilling water pumped from a surface source and tagged with a suitable tracer should be generally identifiable as a contaminant within the bedrock mass by: a) a detectable amount of tracer, b) a surface/near-surface major ion chemistry, and c) detectable amounts of atmospheric derived ^3H and ^{14}C . An absence of (a) but the presence of (b) and (c) would lead one to suspect near-surface derived water transported from its point of origin by natural (recharge) or artificial (excessive pumping during interference testing or during sampling) causes. Similarly, the presence of saline water (i.e. usually of a deep source origin) characterised by an absence of ^3H and low amounts of ^{14}C sampled at a near-surface locality, would tend to make one suspect that groundwaters from depth have found their way to the surface either by natural means (discharge) or again artificially by excessive pumping from other parts of the bedrock or from the borehole by short-circuiting around the packers. In each case additional knowledge of the hydraulic parameters and geology of the borehole section should support or otherwise confirm this initial hypothesis. If it is supported, then further evidence is not required. If not, then another explanation is required. If the hydraulic information is inadequate, then more emphasis has to be put on the borehole geology (i.e. presence or absence of fractures etc.).

2.3 Results

Resulting from the manual classification, the Group I and II site areas (Table 1) showed that only a few of the sampled borehole sections were considered representative, i.e. reflecting in situ groundwater conditions (Smellie et al., 1985, 1987). These samples were from Fjällveden (Fj2: 605 - 607 m), Gideå (Gi2: 178 - 180 m; Gi4: 222 - 224 m), Svartboberget (Sv4: 376 - 378 m) and Kråkemåla (K11: 406 - 564 m). No effort was made to group the remaining "unrepresentative" data.

Using the representative data, an attempt was made to find some common characteristics between these sampled borehole sections. Smellie et al. (1985; Table 6.2) compared the hydrological and geological features of each groundwater environment in the Group I sites. This showed:

- a) At two of the sites (Gideå and Svartboberget) dykes of granite/pegmatite characterised the bedrock either within or near the sampled sections. Similar geological relationships, however, were not reflected at Fjällveden or Kråkemåla
- b) At only two of the five selected horizons considered representative were major local fracture zones involved; the remaining three sections were characterised by normal "background" fracture types
- c) Hydrologically, it was expected that the representative horizons would be characterised by a high hydraulic conductivity coupled with a positive piezometric head, i.e. where

contaminating waters would least be expected to affect the bedrock adjacent to the sampled section. Although this was the case for two of borehole sections in particular, it was not a general feature.

In conclusion, therefore, regarding the Group I and II site areas, there were no significant geological or hydrological features in common with those sections considered representative that could be used as a guideline when selecting suitable sampling sections in future studies. It appeared that every area was hydrogeologically unique, reflecting the importance of the physical properties of the bedrock and the associated fracture geometry resulting from regional tectonic influences.

Group III groundwaters collected from Finnsjön played a central role in assessing new methods (i.e. air-flush percussion) to minimise the contaminating effects of drilling, in addition to characterising the groundwater environment within and adjacent to the highly conductive low-angle fracture Zone 2. This zone represents a horizon along which groundwaters of contrasting age and chemistry come into contact and partially mix. Comparison was made between traditional water-flush core and air-flush methods and their respective effect on groundwater composition. The comparison showed:

- * the limitations of air-flushing; the technique was only efficient down to relatively shallow depths (200 - 250 m)
- * increasing air pressure also serves to extend the radius of groundwater contamination (i.e. oxygen/groundwater dissolution) in the host bedrock along hydraulically active horizons such as Zone 2 (i.e. high conductivity coupled with a negative piezometric head). This resulted in serious changes in pH, Eh and the distribution of redox-sensitive elements
- * in conjunction with a stepwise drilling/sampling procedure, traditional rotary water-flush methods were preferred to minimise groundwater contamination

The Group III samples, collected from the water-flush cored boreholes, were considered to be mostly representative. Even though contaminating water sources (i.e. drilling water and hydraulic test injection water) were introduced into and along Zone 2, the conductivity was such that any contamination remaining after the gas-lift pumping was quickly flushed out of the system. In the less conductive sections, contaminants were removed during gas-lift pumping and during the pre-sampling monitoring period.

As a general rule, the more parameters available (Table 1), the better the prospects for a robust evaluation. In particular, because groundwater flow takes place in a system of conducting fracture zones, some of which may constitute pathways of rapid flow through the bedrock, the importance of quantitative hydraulic data cannot be over-emphasised in evaluating in situ groundwater quality.

2.4 Discussion

The manual classification method as presented here is not based on any specific cut-off limits, whether analytical or otherwise. Hydraulic systems in crystalline bedrock environments are often too complex for such restrictions when groundwater mixing from different sources commonly occurs. Consequently, it was decided that samples are better evaluated against a background of collective parameters which, through a systematic sequence of elimination, eventually judge the sample to be representative or not in terms of in situ groundwater quality. The advantage of this approach is that a large amount of very useful background qualitative information, and not only quantitative data, can be used in the evaluation, e.g. variations of groundwater chemistry during the pre-sampling monitoring stage, the effect of sudden pump failure or excessive pump-rates over long time periods, how the samples were collected, analytical difficulties and reliability etc. The inter-relationships between quantitative and qualitative data often prove to be decisive factors in quality evaluation.

The main drawback to this classification method is that it tends to focus on selecting only the “best” samples, even though this was the primary aim of the exercise. It is relatively easy to set high standards of selection (i.e. tritium or no tritium; drilling water or no drilling water etc.) and there is a danger of being overly selective. Some balance, however subjective, must be maintained. This works satisfactory for local site investigations with a limited amount of data and well defined hydraulic boundaries.

An obvious potential disadvantage is reproducibility; different people may tend to emphasise different parameters. In practice, however, as the overall judgement is based on the interplay of all influencing parameters, the emphasis of one parameter over another tends to be minimised, and a balanced assessment is obtained.

3 USED AND TESTED QUALITY CLASSIFICATION METHODS

3.1 Manual classification of Äspö, Sweden

3.1.1 Background

More recent groundwater quality evaluations have been carried out at the Äspö Hard Rock Laboratory site (Smellie and Laaksoharju, 1992). Äspö differs from the earlier site-specific investigations in that less emphasis was given to detailed downhole hydraulic measurements (Table 1). In this case, a more global hydrogeological conceptual model was required with the result that greater importance was given to extensive large-scale interference pump testing. This has given rise to groundwater mixing and contamination on a much grander scale than in the earlier site studies.

Generally, the following sequence of borehole activities were carried out at the Äspö site subsequent to chemical sampling:

- * borehole clearance using gas-lift pumping coupled with spinner surveys along the entire borehole length
- * pumping tests of the entire borehole
- * geophysical logging of the entire borehole
- * hydraulic injection tests along 3 and 30 m sections
- * based on the above test results, specific hydraulically conductive borehole sections were selected for transient interference tests, and dilution tests were performed on some borehole sections
- * groundwater sampling from isolated sections of approx. 3 - 10 m length

The sequence of activities from drilling to groundwater sampling was not always systematic; groundwater sampling (sometimes only limited to uranine tracer monitoring of the flushing water contents) has been carried out at various occasions in association with drilling, borehole clearance and pump tests etc. At Äspö, drilling and hydraulic testing using near-surface waters (<100 m) may have resulted in direct contamination. Subsequent raising and lowering of geophysical probes may also have caused groundwater perturbation in the boreholes resulting in the mixing of non-saline and saline water types.

Contamination need not relate to major groundwater compositional changes, but may mean re-introducing waters which have mostly undergone pH and Eh changes through degassing and oxidation etc. when pumped to the surface. This is particularly pertinent to the upper 100 m of bedrock at Äspö where the introduced drilling and hydraulic testing waters are essentially derived from the same bedrock depth. At greater depths, where the formational groundwaters are highly saline, such borehole activities effectively introduce a near-surface, non-saline component into the most conductive zones intercepted by the boreholes.

Open hole effects may also contribute to a general mixing of groundwater types in the borehole; in the case of Äspö the mixing of non-saline with saline has posed the greatest problem in interpretation. The degree of mixing will depend on the hydraulic properties of the borehole and possibly on groundwater density variations.

3.1.2 Method

Initially the Äspö data were evaluated along similar lines to those described above for the earlier site-specific studies. Using the various parameters listed in Table 1, the groundwater chemical and isotopic trends were evaluated and classified resulting in a choice of “representative” and “non representative” in situ groundwater types. However, because of the absence of reliable hydraulic data, it was not possible to calculate the water budgets so that more reliance was put on those parameters of greatest influence, namely the presence or absence of tagged borehole activity water and tritium, and on the groundwater extraction rates (Table 2). By applying these parameters, it has been possible to present a more strict appraisal of groundwater response at Äspö.

One drawback with evaluating the groundwater quality at Äspö is that in several cases the extraction pump-rate chosen for hydraulic interference testing of the boreholes was, naturally enough, based on hydraulic and not hydrogeochemical criteria. Consequently, and depending on the hydraulic properties of the interconnected conductive zones, groundwaters have been removed for chemical analysis which are a mixture of waters from varying levels and origins in the bedrock. In addition, at high flow rates it is not possible to accurately measure important parameters such as the redox potential. For hydrogeochemical purposes, therefore, the lower the extraction rate the less perturbation of the system and therefore the closer one can approach the natural groundwater conditions.

3.1.3 Results

The results of the manual classification of the Äspö waters are shown in Table 2.

Table 2. Classification of sampled groundwaters from Äspö.

Borehole/section (m)	Representative		Non Representative			
	Criteria A	Criteria B	Criteria C	Criteria D	Criteria E	Criteria F
KAS02:202 -215	x					
KAS02:308 -344	x					
KAS02:314 -319		x				
KAS02:463 -468			x			
KAS02:530 -535	x					
KAS02:802 -924		x				
KAS02:860 -924		x				
KAS03:129 -134	x					
KAS03:196 -223				x	x	
KAS03:248 -251		x				
KAS03:347 -374		x				
KAS03:453 -480				x	x	
KAS03:609 -623					x	
KAS03:690 -1002				x	x	
KAS03:860 -1002	x				x	
KAS04:226 -235			x			x
KAS04:334 -343	x					
KAS04:440 -481			x			
KAS06:204 -277				x		x
KAS06:304 -377	x					
KAS06:389 -406				x		
KAS06:439 -602				x		x
HAS13:0-100				x		x

Criteria:
A = Representative groundwater for the sampled isolated level (Assumed limited sampling radius because of the low extraction pump-rates: <200 mL/min).
B = Representative groundwater for the sampled isolated level (Assumed large sampling radius because of the high extraction pump-rates: 1500 to 18800 ml/min).
C = Non-representative groundwater at low extraction pump-rates.
D = Non-representative groundwater at high extraction pump-rates.
E = Containing borehole activity water (>1% uranine).
F = Containing a young (<45 a) groundwater component (>2 TU)

3.1.4 Discussion

The results of the manual classification of the Äspö waters are shown in Table 2. The table shows that most of the representative samples were, as expected, collected at low extraction rates (A), and the three not regarded as suitable (C) was mainly due to short circuiting of borehole water from higher bedrock levels (e.g. at level 226 - 235 m in KAS04; this was corroborated by the presence of tritium and major ion chemistry). Short circuiting resulted from the choice of a borehole section of very low hydraulic conductivity, such that, even at the low extraction rates used (<200 mL/min), there was inadequate borehole recharge groundwater available from the packed off sections.

Most of the non representative samples are a product of high extraction rates (D) coupled to either excess tagged activity water (E) or excess tritium (F). Nevertheless, several representative groundwater samples resulting from high extraction rates have also been

reported (B). This indicates access to aquifers in the near vicinity of the selected borehole sections which are highly conductive and are not directly hydraulically connected with excessively shallow or deep groundwater sources.

The correlation between some high extraction rates and a non representative groundwater sample is of no great surprise at Äspö. From the hydraulic investigations several large-scale water conducting fractures control the groundwater flow through the island. Interference tests have shown the interconnection between these zones, some recharging (e.g. NNW-trending vertical to sub vertical fracture zones), some discharging (e.g. sub vertical zone NE-2). High extraction rates, in some cases, will obviously force in groundwaters from shallow and/or deeper bedrock levels, depending on borehole location and which fracture zones are intercepted and the hydraulic properties of those zones.

Treated individually, the data presented in Table 2 may not appear too promising. However, from detailed studies it is possible to know with reasonable certainty the origin of the groundwaters, at low extraction rates, that have been short circuited (e.g. type "C"). This has played an important role in establishing the levels of groundwater mixing and also in explaining some of the discrepancies (i.e. pH and Eh) in the water/rock chemical equilibrium modelling. At high extraction rates this detective work is more difficult, but nevertheless the major ion fluctuations have been extremely useful in helping to construct the conceptual groundwater flow model (Smellie and Laaksoharju, 1992).

Table 2 should, therefore, be regarded as an interpretative guide to any study which involves a groundwater medium, where different levels of accuracy are required. For example, colloidal, organic and microbial studies require a high degree of finesse with regard to origin, groundwater chemistry and transport pathways. In these cases, well defined sampling sections at low extraction rates are of paramount importance. For other studies, such as major ion groundwater geochemical evolution and large-scale groundwater flow paths, all chemical information at both low and high extraction rates are important.

3.2 Manual disturbance test of Finnish groundwater data

3.2.1 Background

TVO site investigations

TVO (Teollisuuden Voima Oy) performed preliminary site investigations from 1987 - 1992 at five areas; Romuvaara, Veitsivaara, Kivetty, Syry and Olkiluoto. In addition to groundwater chemistry (see Lampén and Snellman, 1993), investigations at the sites included geology, hydrology and geophysics. Altogether 340 water samples were collected comprising: a) shallow water environmental reference samples from brooks, lakes, natural springs, domestic wells, precipitation and snow, b) groundwater samples from deep drilled boreholes (maximum 1000 m deep), and c) groundwaters from downhole multilevel piezometers installed for hydrological investigations. The drilling flushing water used was generally taken from a local shallow borehole.

Groundwater sampling from the deep boreholes was carried out using two separate sets of pumping equipment. TVO's equipment (Öhberg, 1991; Rouhiainen et al., 1992) operates at a low pumping rate, usually less than 300 mL/min, and the water samples are collected from borehole sections isolated with inflatable packers. On-line, in situ chemical field measurements were performed at the surface using a combination of several flow-through cells. Groundwater samples were also taken with a high capacity submersible pump used for hydrological pumping tests.

The representativeness of the groundwater samples has been evaluated in the field based on the remaining amount of flushing water present, commonly labelled with two tracers: uranine and iodide. Furthermore, field measurements of Eh, dissolved O₂, pH, pS, electrical conductivity and temperature give some idea of the overall trends in the chemistry during the pumping. The quality of the laboratory analyses is estimated using charge balance calculations. The hydrogeochemical site investigations have been described and discussed by Lampén and Snellman (1993).

IVO site investigations

IVO (Imatran Voima Oy) has been involved since the end of the 1970's in bedrock studies from the Hästholmen area. Groundwater samples from Hästholmen, collected from 1980 - 1983, were sampled employing a downhole double packer system; the water was pumped to the surface using an over pressure of nitrogen. Unfortunately, the nitrogen flushing of the water has particularly influenced pH, alkalinity and other gas-sensitive parameters. Furthermore, during bottling of the samples atmospheric contamination cannot be ruled out. Atmospheric contact has also rendered doubtful the reliability of the field measurements (e.g. pH, Eh, O₂), even though they were performed under a short period of time. Consequently, these measurements have not been included in the 1980 - 1983 Hästholmen data set.

Sampling from 1985 - 1992 was performed using TVO's double packer equipment, and field measurements of Eh, pH, pS and dissolved O₂, temperature and electrical conductivity were measured in a flow-through cell. Direct contact with nitrogen gas or air was eliminated. These samples are considered the most representative of the Hästholmen samples; unfortunately, due to technical problems no redox measurements were recorded during the first sampling event in 1985.

The flushing water contamination at Hästholmen, estimated on the basis of the tritium content, is less in the deep saline water (0 - 30%) than observed in the near-surface fresh water layer (30 - 74%). However, since the undisturbed in-situ tritium value in the section is unknown, these calculations indicate the maximum possible (but probable) contamination.

The accuracy of the laboratory analyses was evaluated by charge balance calculations. These showed that some 85% of the total 150 samples fell within the +/-10% charge balance range. The hydrogeochemical site investigations of Hästholmen are discussed more thoroughly by Snellman and Helenius (1992).

3.2.2 Method

Using the TVO hydrogeochemical database a manual system to test for groundwater disturbance effects was developed to estimate the influence of drilling, borehole activities, groundwater sampling and surface water contamination. The system mainly emphasises the direct contamination of shallow and deep groundwaters by near-surface water input. It should be noted that the suggested system is not a standard quality classification method, where useful and unsuitable data are grouped, but rather only indicates the influence of one (or more) measured contaminant parameters found in near-surface waters (Table 3).

Table 3. Disturbance parameters considered.

Sampling	Contamination	Analytic	Near-surface Water
pump-rate	TOC	charge balance	³ H
Eh(field)	KMnO ₄		TOC
O ₂ (field)	NO ₃		KMnO ₄
drill water	NH ₄		NO ₃
	PO ₄		NH ₄
			PO ₄

Most of the boundary values for these near-surface water parameters were selected from established drinking water standard limits given by the Finnish National Agency for Wealthfare and Health (Lääkintöhallitus, 1991). These limits (Table 4) have been chosen to specifically describe the effects of surface water and other anthropogenic contamination effects on shallow and deep groundwaters.

Table 4. Near-surface water boundary values used to test disturbances in shallow and deep groundwater samples.

Parameter	Limit / Dimension
³ H	< 8.5 TU
drill water	< 10 %
charge balance	< ± 10 %
Eh (field)	< 0 mV
O ₂ (field)	< 0.5 mg/l
TOC	< 3.5 mg/l
KMnO ₄	< 12 mg/l
NO ₃	< 25 mg/l
NH ₄	< 0.5 mg/l
PO ₄	< 0.1 mg/l

By using a strict cut-off of the near-surface water boundary values (e.g. higher or lower values etc.), and in some cases introducing an additional potential variable of influence, the extraction pump-rate, several criteria were identified (Table 5). These criteria corresponded

to different disturbance categories of the groundwaters which, for simplicity, are classified as surface and shallow (0 - 100 m) and deep (100 - 1000 m). These disturbance criteria were applied to the hydrogeochemical data (Table 6).

Table 5. Disturbance test criteria used for shallow and deep groundwater samples.

Disturbance category	Criteria
A (deep groundwater)	- groundwater with all of the listed parameters lower than the boundary values (Table 4). - the sample has been collected with a low pump-rate (<300 ml/min).
B (deep groundwater)	- groundwater with all of the listed parameters lower than the boundary values (Table 4). - the sample has been collected with a high pump-rate during hydrotests (>>300 ml/min).
C (deep groundwater)	- groundwater with at least one of the parameters exceeding the boundary value (Table 4).
D (surface and shallow water)	- the values of TOC, KMnO_4 , NO_3 , NH_4 , PO_4 and charge balance in the surface and shallow water are lower than the boundary values listed in Table 4.
E (surface and shallow water)	- at least one of the parameters exceeds the boundary value (Table 4).

3.2.3 Results

The disturbance test criteria listed in Table 5 resulted in the classification shown below in Table 6. The table shows the number of samples considered undisturbed; these are related to the investigated site location and to the type of sample, i.e. surface precipitation, near-surface and shallow wells sources and deep groundwaters from boreholes using specialised equipment (e.g. inflatable packers etc.). The pump-rate has also been considered.

Table 6. Number of "undisturbed" samples at the different sites.

Type of Water samples	Romu-vaara	Veitsi-vaara	Kivetty	Syry	Olki-luoto	Häst-holmen
Environmental reference samples (ENV)	-	3	5	2	1	-
Precipitation and snow samples (RAIN, SNOW)	3	2	7	7	3	-
Samples from the flushing water wells (KA)	-	-	4	-	-	-
Drillholes sampled with TVO's equipment (KR)	-	-	-	-	-	-
Drillholes samples with high pump-rate during hydrological pump tests (KR*)	-	-	7	-	-	-

3.2.4 Discussion

According to the classification summarised in Table 6, at Kivetty only the shallow well near-surface waters and the deep groundwater samples from the hydraulic pumping tests, together with some environmental reference, rain and snow samples, can be considered undisturbed and therefore representative. The result from Kivetty is consistent with the geochemical interpretation which considered the final samples collected during the hydraulic pumping tests from the level 808 m to represent mature groundwater (Pitkänen et al. 1992a). The geochemical interpretation of the Syry groundwaters, whilst supporting undisturbed and representative samples from the uppermost sampling levels of borehole KR1, also indicate undisturbed samples from the lowermost level at 739 m, which is not indicated in Table 6. There is geochemical support for undisturbed samples at Syry, despite the high percentage of drilling water contamination (Pitkänen et al. 1990). Geochemical modelling of the Olkiluoto groundwaters suggests that the samples from KR2 are not representative (in agreement with Table 6), due to the influence of surface water and possibly also by cement from the overburden section of the borehole. This is clearly indicated by high values of pH, HCO_3 , pCO_2 and ^3H . The brackish groundwaters at both Syry and Olkiluoto reflect mixing with a relict Baltic sea water component. In addition, saline groundwaters are believed to contain a considerable component of old water, possibly of hydrothermal origin.

The frequency of those parameters which have resulted in the rejection of water samples from Kivetty and Olkiluoto sites have been tested and are shown in Figures 4 and 5.

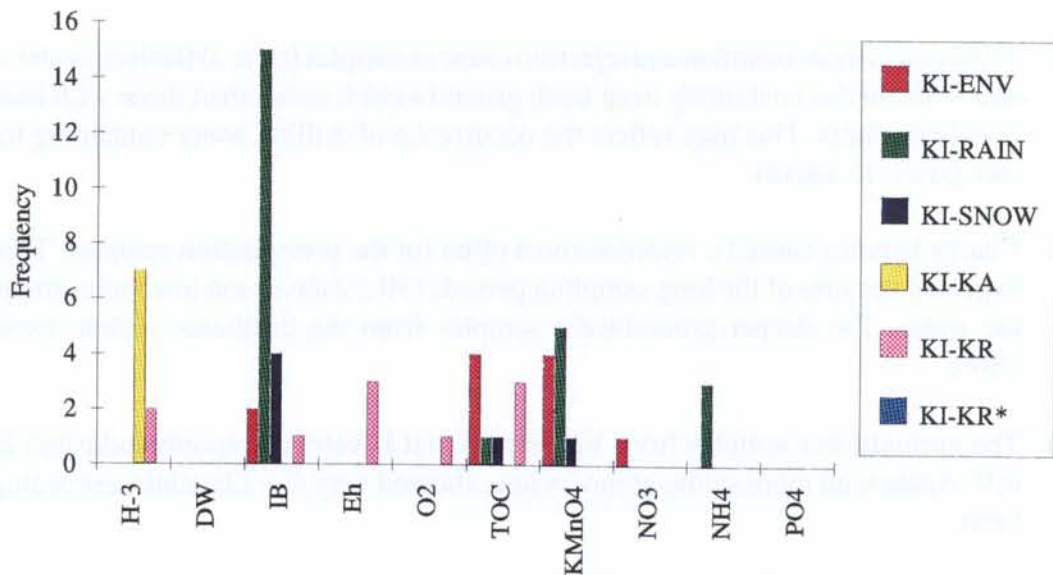


Figure 4. Disturbance test of the Kivetty (KI) water samples. Increasing bar length indicates the frequency of those parameters exceeding the boundary limits as listed in Table 4. (DW = Drilling water, IB = Charge balance, KA = flushing water well sample, KR = Packer equipment sample, KR* = Hydrotest sample).

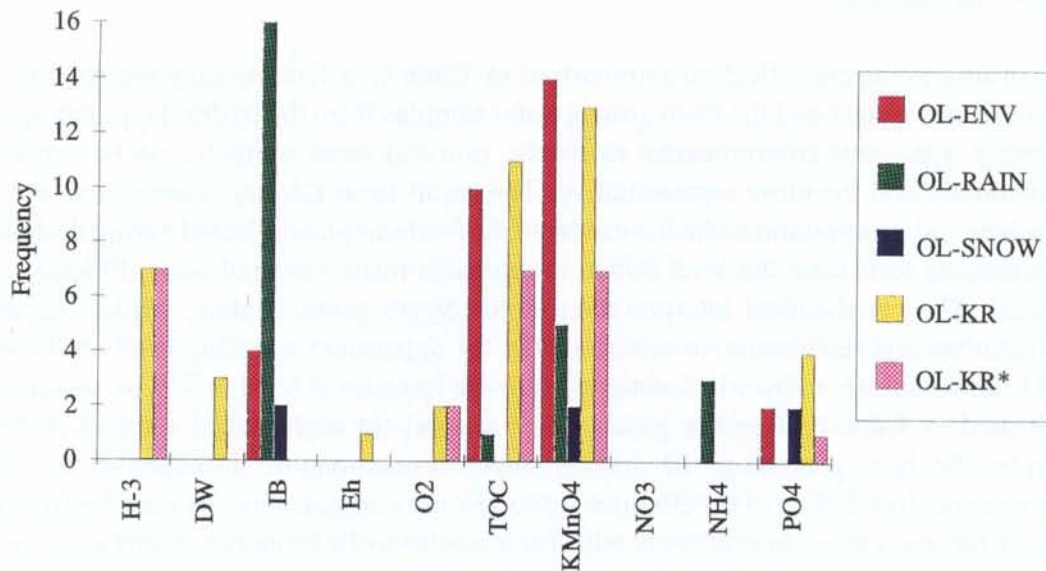


Figure 5. Disturbance test of the Olkiluoto (OL) water samples. Increasing bar length indicates the frequency of those parameters exceeding the boundary limits as listed in Table 4. (DW = Drilling water, IB = Charge balance, KR = Packer equipment sample, KR* = Hydrottest sample).

The following general trends can be observed from the data:

- 1) Drilling water was a more common rejection cause in areas characterised by brackish and saline groundwaters.
- 2) Tritium was more common as a rejection cause in samples from: a) flushing water wells, and b) drillholes containing deep fresh groundwaters, rather than those with brackish or saline waters. This may reflect the occurrence of drilling water containing tritium (see point (1) above).
- 3) Charge balance caused a rejection most often for the precipitation samples. This was expected because of the long sampling periods (30 ± 2 days) and low ionic strength of the water. The deeper groundwater samples from the drillholes seldom exceeded $\pm 10\%$.
- 4) The groundwater samples from Veitsivaara and Kivetty commonly indicated $Eh > 0$ mV. Areas with more saline groundwaters showed very few Eh values exceeding this limit.
- 5) The deeper groundwaters from Romuvaara, Veitsivaara, Syyry and Olkiluoto showed significant dissolved oxygen contents ($O_2 > 0.5$ mg/L) due to contamination and disturbances in the flow-through cell in the field.
- 6) Some water samples from areas characterised by fresh deep groundwaters (Romuvara, Veitsivaara and Kivetty) and many samples from more saline areas (Syyry and

Olkiluoto) showed increased TOC (>3.5 mg/L). The latter observation might reflect analytical problems due to the high salinity.

- 7) In some cases KMnO_4 (concentration >12 mg/L) was a general rejection cause in the fresh deep groundwater areas, and a common rejection cause at Syyry and Olkiluoto where KMnO_4 is present in samples representing both surface and groundwaters. The high KMnO_4 values were generally confirmed by high TOC values.
- 8) NO_3 was a rejection cause only in some surface water samples ($\text{NO}_3 > 25$ mg/L). These were always caused by anthropogenic factors, such as farming or agriculture.
- 9) NH_4 was observed to be a rejecting cause in some precipitation samples from Romuvaara and Kivetty. This is probably due to the long sampling period which allows deterioration. In addition, some surface samples from Syyry and Olkiluoto also showed elevated amounts of NH_4 (>0.5 mg/L). Again antropogenic factors were observed. Deep groundwater samples from Hästholmen showed elevated amounts of NH_4 thought to be due to contamination from the washing of the sample bottles or other equipment.
- 10) The limit of PO_4 was set to 0.1 mg/L. Surface waters from nearly all the TVO investigation areas showed some elevated values. At Romuvaara, Olkiluoto and Hästholmen borehole samples showed anomalous values; at Hästholmen, contamination due to detergents was suspected.

The sensitivity of the redox system to groundwater disturbance is well known and can be demonstrated with the help of redox-sensitive parameters such as Eh, O_2 , $\text{Fe}^{2+}/\text{Fe}(\text{tot})$ and the occurrence of reducing gases (CH_4 , H_2). By using these parameters and some additional boundary criteria, the redox observations can allow subdivision into disturbed and less disturbed conditions as outlined in Table 7.

The difficulties of obtaining less disturbed groundwater Eh-values are well known. However, the influence of, for example, leakage, short pumping periods, excessive use of flushing water etc. (Table 7), show that aspects other than the chemistry of the groundwater can influence redox measurements. The listed disturbances in Table 7 have generally occurred prior to water sampling. In some cases, however, the effects of the disturbance, for example changes in the pH values, may be mathematically corrected to reflect in-situ conditions (Pitkänen et al., 1992b).

Disturbed, although still reducing groundwater conditions, were generally obtained in the sampling from Kivetty (borehole KR1) and Olkiluoto (boreholes KR1, KR2, KR3 and KR5) as well as at Veitsivaara (borehole KR4), Romuvaara (borehole KR5) and Syyry at the uppermost sampling depth (borehole KR1) and from boreholes KR2 and KR6. Less disturbed reducing conditions were obtained in Syyry at the depths below 600 m (borehole KR1) and Romuvaara (borehole KR1) at a depth of 645 m and at Olkiluoto (borehole KR1) at a depth of 140 m.

Table 7. Disturbed and less disturbed conditions produced when sampling and measuring redox-sensitive parameters and elements.

Conditions	Sampling	Chemical analyses	Dissolved gases	Disturbances
Disturbed	Eh(field) < 0 mV 0,05 mg/L < O ₂ (field) < 0,5 mg/L	0,5 < Fe ²⁺ /Fe(tot) < 1,0 possible occurrence of HS ⁻	O ₂ < 5 % (vol.) with possible occurrence of H ₂ and CH ₄	- recent calibration - valve leakage - pump breaks - a short pumping period - slow pump-rate - lots of flushing water
Less-disturbed	Eh(field) < -100 mV O ₂ (field) < 0,05 mg/L	Fe ²⁺ /Fe(tot) = 1 occurrence of HS ⁻	occurrence of reducing gases (CH ₄ , H ₂)	

Summary

The described sorting system concerns parameters which indicate possible contamination caused by drilling or other borehole activities resulting in the mixing of surface or shallow waters with deeper groundwaters, or other, possibly anthropogenic sources of contamination such as agriculture chemicals. However, despite the results of this rather rigid and strict classification, the disturbed samples can still be used. The major components and the less sensitive parameters are often unaffected and reflect the principal features of the local bedrock groundwater interaction system. These data have therefore been used in the hydrogeochemical characterisation of the investigation sites in Finland and in a general comparison between the sites. The samples are also used for water evolution and water type classification developed by Davis and De Wiest (1967), since this method only uses major element components. Recent groundwater investigations in Finland have thoroughly discussed the representativeness of groundwater samples (Lampén et al., 1992).

The advantage of this approach is the clear response to contamination from different possible sources expected to occur in hydrogeochemical site investigations. One disadvantage is the rigidity of the system, since the disturbance response caused by one parameter is enough to reject the sample. However, the rejected data can still be used for the purposes discussed above. In future this sorting system could also be developed to consider the weight of different parameters.

3.3 Statistical classification

3.3.1 Background

In order to base groundwater quality evaluations statistically, and thereby objectively, attempts were made to apply a multivariate analytical approach to groundwater classification. Multivariate analyses (MV) are used to identify or model the character of analytical data; the strength of this approach is that several or all variables in a data matrix can be

examined simultaneously. The character of the data in a general data matrix is therefore more easily identified than using univariate analysis, where only one variable is compared at a time (Wold, 1987). With multivariate analysis, data can be explored, minimised, structured, correlated and classified. The underlying theme of much multivariate analyses is simplification. The computer code STATGRAFICS (1991) version 5.0 from STSC has been used in the description below.

MV deals with Objects (samples) described by Variables (chemical quantities), and searches to establish the relationship between objects, between variables, and between objects and variables. Objects and variables can be equal, similar, dissimilar, proportional, mixtures and linear combinations. MV attempts to address the following: that objects 1, 2 and 3 are equal or similar, that objects 4 and 5 are equal or similar, but dissimilar from objects 1, 2 and 3. Linear or complex relationships are possible between one variable and some other variable(s) or object (Mardia et al., 1979).

3.3.2 Method

Groundwater modelling using multivariate analysis involved data from the Äspö studies in Sweden (Smellie and Laaksoharju, 1992) and initially concentrated on classifying or categorising the groundwaters by simplifying the analytical data. The questions posed were: a) which are the most useful chemical variables?, b) which variables are insignificant?, c) can the method be used for quality control of the samples? During the modelling of Äspö data several MV-techniques were found to be useful.

Correlation Analysis

In Correlation Analyses connections and disconnection between the variables and observations are detected. The Correlation Analysis procedure generates a matrix of correlation coefficients for a set of observed values. Correlation Analysis often provides a preliminary view of the relationships among variables. For example, the correlation between the sampling method and the measured chemical values was investigated.

Correlation coefficients provide a normalised and scale-free measure of the linear association between the variables. The coefficient values fall between -1 and +1; a positive correlation indicates that the variables vary in the same direction while a negative correlation indicates that the variables vary in the opposite direction. Statistically independent variables have an expected correlation of zero.

The results from the Correlation Analysis procedure can be used as input for some procedures such as principal component and factor analysis.

Principal Component and Factor analysis

With Principal Component Analysis and Factor Analyses the main aim is to replace the original variables by a smaller number of “underlying” variables. The idea is to derive new variables which will hopefully give a better understanding of the data.

Principal Component Analysis consists of finding an orthogonal transformation of the original variables to a new set of uncorrelated variables (Chatfield and Collins, 1989). This transformation consists of a rigid rotation or a rotation plus reflection preserving the distances and angles in the matrix. The new variables are called Principal Components, which are linear combinations of the original variables. The components are derived in decreasing order of importance. Generally the first few components will account for most of the variation in the original data so that the effective dimensionality of the data can be reduced and hence the information simplified.

Factor Analysis has a similar aim but instead of a pure mathematical model a proper statistical model is applied to the data, which specifies a given number of underlying variables called factors. The analysis is more focused on the covariance or similarity of the variables rather than the variance or variability as described above in the Principal Component Analysis.

Using these techniques the importance or usefulness of different variables can be tested. For example, by employing this method, Cl, Na, Ca, SO₄ and HCO₃ can be shown to describe most of the variability in the chemistry data (Laaksoharju, 1990). These components are therefore generally used in classifying groundwater types.

Multivariate Control Charts

Multivariate Control Charts are used to test those observations of lowest quality compared to the others, based on some quality indicating variables obtained using the previous methods. This method can handle slight simultaneous shifts in several variables, which may not attract attention unless all variables are considered together. The procedure allows one to construct control charts (based on the statistical Hotellings T-squared method) in which different measurements can be correlated. The procedure transforms the original correlated variables into new variables that are independent and then constructs a single statistic based on the new variables. The system then plots the observations on a single control chart with an upper limit; observations beyond the limit are considered in this specific application to be of inferior quality.

3.3.3 Results

Correlation Analysis were carried out on the Äspö data (Smellie and Laaksoharju, 1992) to detect any relationship between the sampling methods employed (non chemical variables) and the groundwater compositions (chemical variables). The chemical variables used were: a) major element chemical analyses, b) isotope analyses, and c) residual drilling water component, and the non chemical variables were a) extraction pump-rate, b) piezometric head, and c) sampling method (open hole, inflatable packers etc.). Using Correlation- and Principal Component-Analysis only three variables have shown to be of importance; *stable isotopes* (²H and ¹⁸O), *extraction pump-rate* and *sampling method*.

Using the Multivariate Control Chart method, the so-called T-squared values for the three correlating variables were calculated. The control chart is illustrated in Figure 6; the higher the value the lower the quality of the integrated variables, i.e. the less representative the groundwater quality. With the exception of samples KAS02:308/463/530, KAS03:129/196 and possibly KAS04:334, all the remaining samples suggest a lack of representativeness, in particular KAS02:802, KAS03:248 and KAS06:389/439.

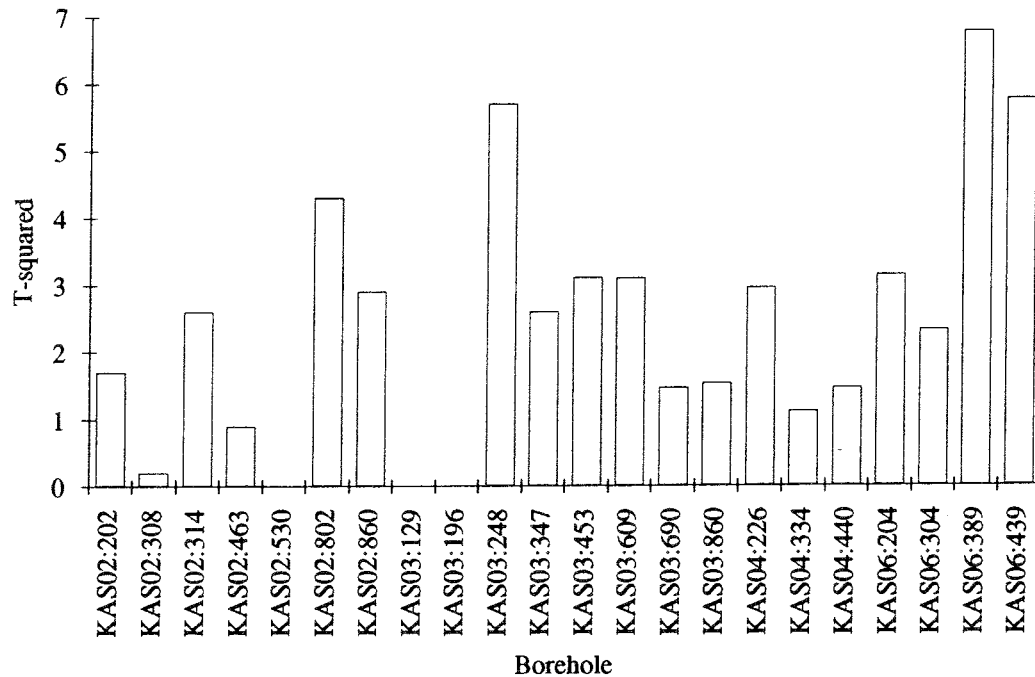


Figure 6. Results of the multivariate control chart method on the Äspö borehole data. The higher the relative Hotellings T-squared value the lower the groundwater quality.

3.3.4 Discussion

The results of the multivariate classification shown in Figure 6 allocate, for example, a low quality for KAS03:248m. Interestingly, this observation was classified as representative in the manual classification (Smellie and Laaksoharju, 1992; also section 3.1). This general discrepancy can therefore illustrate the problems encountered when comparing different classification methods. Perhaps the fault lies in the choice of emphasis, for example, in the manual classification, known risk factors such as drilling water and pump extraction flow-rate are emphasised, whilst in the MV-method the stable isotopes are also considered as being equally important. Furthermore, the MV-method reflects the weighted response in some of the selected and statistically tested chemical variables measured. Therefore, the conclusion at this point in the study was that the application of Multivariate Analyses, because of the high resolution and reproducibility, should be further evaluated.

Refinement of the MV-method

The next approach was to find any additional correlation between chemical variables and different non-chemical variables that could have affected the quality of the waters. The use of the following chosen variables were tested (Table 8):

Table 8. Comparison of multivariate strategy to evaluate the quality of the groundwater.

Quantitative Parameters	Semi-quantitative Parameters	Descriptive Parameters
Major/minor ions: HCO ₃ , Cl, Br, SO ₄ , PO ₄ , NH ₄ , Na, K, Ca, Mg etc.	Pump-rate	Open hole effect
Field measurements: pH, Eh, cond., temp, dissolved O ₂	Water budget: Drilling water, hydrotesting, open-hole effects	Adjacent hole(s)
Redox-sensitive: Fe(tot), FeII, S, Mn, U	Sampling methods: 1) downhole (in-situ Eh & pH) 2) surface (Eh, pH) 3) during hydrotesting 4) open-hole tube sampler 5) simplified, portable sampler	On-going, nearby, site investigation
Isotopes: ² H, ³ H, ¹⁸ O, U-series		Regional pump-tests
Analytical: Charge balance		Drilling activities
Drilling water: Uranine and iodide		Groundwater sampling

In Table 8 three subdivisions have been recognised: quantitative, semi-quantitative and descriptive parameters. The quantitative and descriptive parameters are fairly straight forward, the former including those variables which are directly measurable, and the latter including those variables which are too complex to mathematically constrain. The semi-quantitative parameters, on the other hand, are those which may be addressed mathematically, for example, the sampling method can be allocated a number and, if the drilling and hydrotesting protocols are known and hydrogeology is well characterised, the water budget can be calculated for each borehole and each borehole section sampled. By combining the pump extraction rates with the hydrogeological data (if available), the local widespread effects of pumping may be semi-quantifiable on a local scale. The approach was tested on data from Finnsjön (see data source in Smellie and Wikberg, 1991); however little or no correlation was found. Further classification based on this approach was therefore abandoned.

The main limitation with MV-methods is the lack of quantifiable parameters and, those that can be quantified, are not always available. An added limitation occurs when scaling from a local site-specific to a more regional classification. Parameters routinely measured at a local scale are generally not carried out in regional scale studies (Table 9). This results in "gaps" in the input data table thus weakening or lending bias to the results. The main advantage of the standard MV approach is the reproducibility of the results.

Table 9. Comparison of available information when scaling from local to regional classification.

Local classification, many quality indicating variables:	Regional classification, few quality indicating variables:
Complete chemical characterisation, drilling water, isotopes, hydrogeological parameters etc.	Depth, pH, Ca, Na, HCO ₃ , Temp, Cl, SO ₄ , Electrical conductivity

Summary

The MV-method seems to be more useful on a local site-specific scale where high resolution can be achieved. However, the small data set may cause problems since the number of observations may be insufficient to create a correct model and may cause accidental and erroneous relationships. This may be one of the reasons for the discrepancy when the results are compared with manual classification. The method is probably most effective when confronted with large data sets containing a more complete set of quality indicating variables, quantitatively measured. But since this is not the case with the selected Finnsjön data, and rarely for most site investigations, the variables should first be treated mathematically before using MV-analyses. For example, high tritium values in shallow water are normal but more unnatural in deep waters. This can either be expressed as a quotient (e.g. $^3\text{H}/\text{depth}$) or a boundary value (e.g. $<2 \text{ } ^3\text{H}$) which describes the natural behaviour or an assumed limit of importance selected to describe groundwater quality.

Common with all these models is the necessity to make assumptions which in turn lead to errors that may weaken the resolution of the method. The usefulness of the MV-method for groundwater quality classification has probably yet to be fully realised.

3.4 Classification based on mixing

3.4.1 Background

The water from Äspö was further classified by means of a simple mixing model. Within the Swedish programme groundwater sampling from isolated borehole sections usually includes the collection of a sequence of several samples over a time period of around 1 - 2 weeks prior to the main sampling interval, in addition to the main sampling interval. During this period the ion concentration of the sampled water can increase, decrease or be constant. The dilution or concentration of the water indicates mixing of foreign water types from different sources; in this situation a mixing model can be applied. In a situation where the water composition shows no changing trends, a mixing model cannot obviously be applied.

In groundwaters Cl is a water conservative element and can therefore be used as a tracer to establish degrees of mixing provided the concentrations are great enough. Äspö fulfils this requirement. The changes in the water composition are best described by the concentrations

of Cl, Na, Ca, SO₄ and HCO₃, which are generally analysed for all samples and are therefore useful for the purpose. The first sample collected (first end-member) from the sampling sequence, is mixed with the last sample (second end-member). The content (Cl, Na, Ca, HCO₃, SO₄) from each of these two end-members was then mixed in portions necessary to systematically achieve the measured Cl contents of the other samples from the section. The higher the deviation (expressed as standard deviation, STD) from the model, the less mixing is involved. In such a case the water sample is considered representative for the sampled section and, potentially, should be of a higher quality.

3.4.2 Method

The following procedure was used; mixing ratio calculations (Eq#1) followed by deviation calculations (Eq#2). The final calculation (Eq#3) results in a quality index rating for the sample. The former describes the necessary portions of water needed from the both end-members to achieve the Cl content measured in the new samples. The latter is used to predict new values for Na, Ca, HCO₃, SO₄ and Cl. The predicted values are then compared to the measured values expressed in relative deviation (%). Little or no deviation from the model predictions indicates that the concentration can be adequately explained by mixing; large deviations indicate sources or sinks for a particular element that are not accounted for by the mixing model. The reason for the deviation is regarded as an indication of minimum mixing and a high quality sample. The deviation is equal to the quality index (Eq#3), and high values indicate high quality. The mixing ratio and the deviation is calculated according to the following:

$$\text{Mixing Ratio} = (X-A)/(B-A) \quad \text{Eq\#1}$$

X = measured Cl concentration

A = measured Cl concentration of the last sample

B = measured Cl concentration of the first sample

The relative deviation from the mixing model for respective elements is calculated according to the formula:

$$\text{Relative Deviation (STD)} = (A-(B*C + D*E))*100/A \quad \text{Eq\#2}$$

where:

A = measured element concentration in the investigated sample

B = mixing ratio for the first sample

C = measured element concentration for the first sample

D = mixing ratio for the last sample

E = measured concentration for the last sample

The quality index is equal to the relative deviation according to the formula:

$$\text{Quality Index} = \text{Relative Deviation (high value indicates high quality)} \quad \text{Eq\#3}$$

3.4.3 Results

This mixing model was applied and tested using the Äspö data; the resulting classification is shown in Figure 7. The higher the value the greater the quality and hence the lower the risk that mixing has occurred.

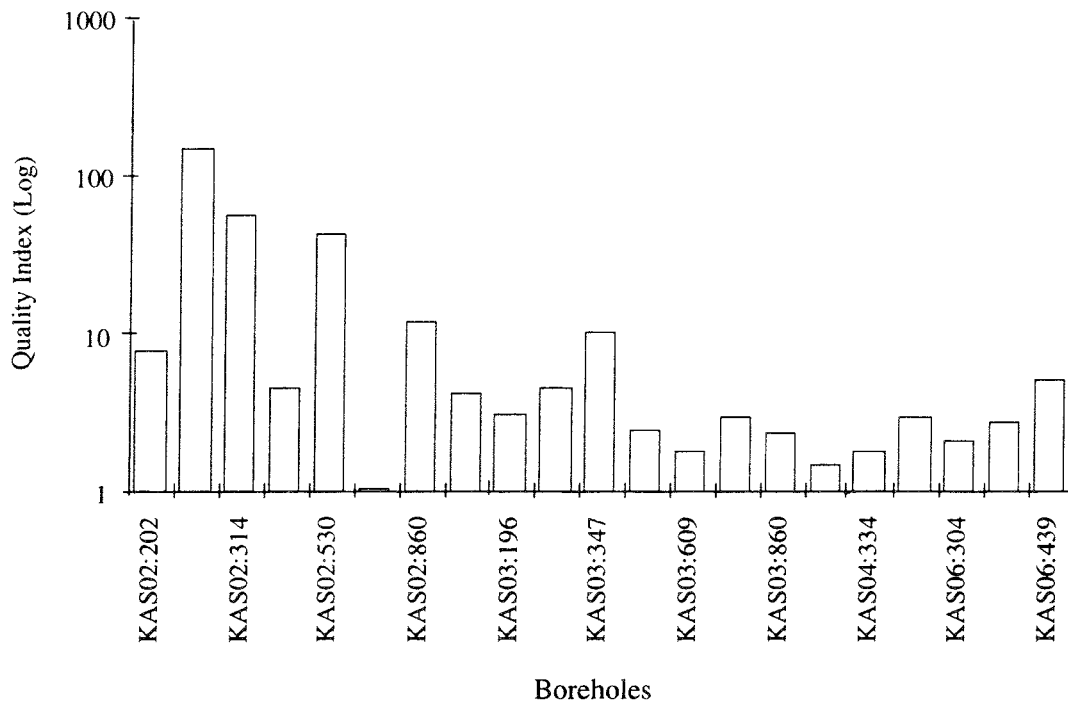


Figure 7. The quality index values are shown for different borehole depths (m). High value indicates good quality.

3.4.4 Discussion

When comparing the results with manual classification the most striking difference is KAS02:802 where the calculations suggests a high mixing risk sample of low quality and therefore not representative for the sampled location. Contrastingly the manual classification (section 3.1) indicated a high degree of representativeness. The most likely reason is that two completely different approaches have been used.

The reliability of mixing model calculations was tested by plotting the quality indices against some known quality indicating variables such as; TOC, pump-rate, drilling water and charge balance (Fig. 8). High quality index values indicate high quality and minimum mixing of the sample.

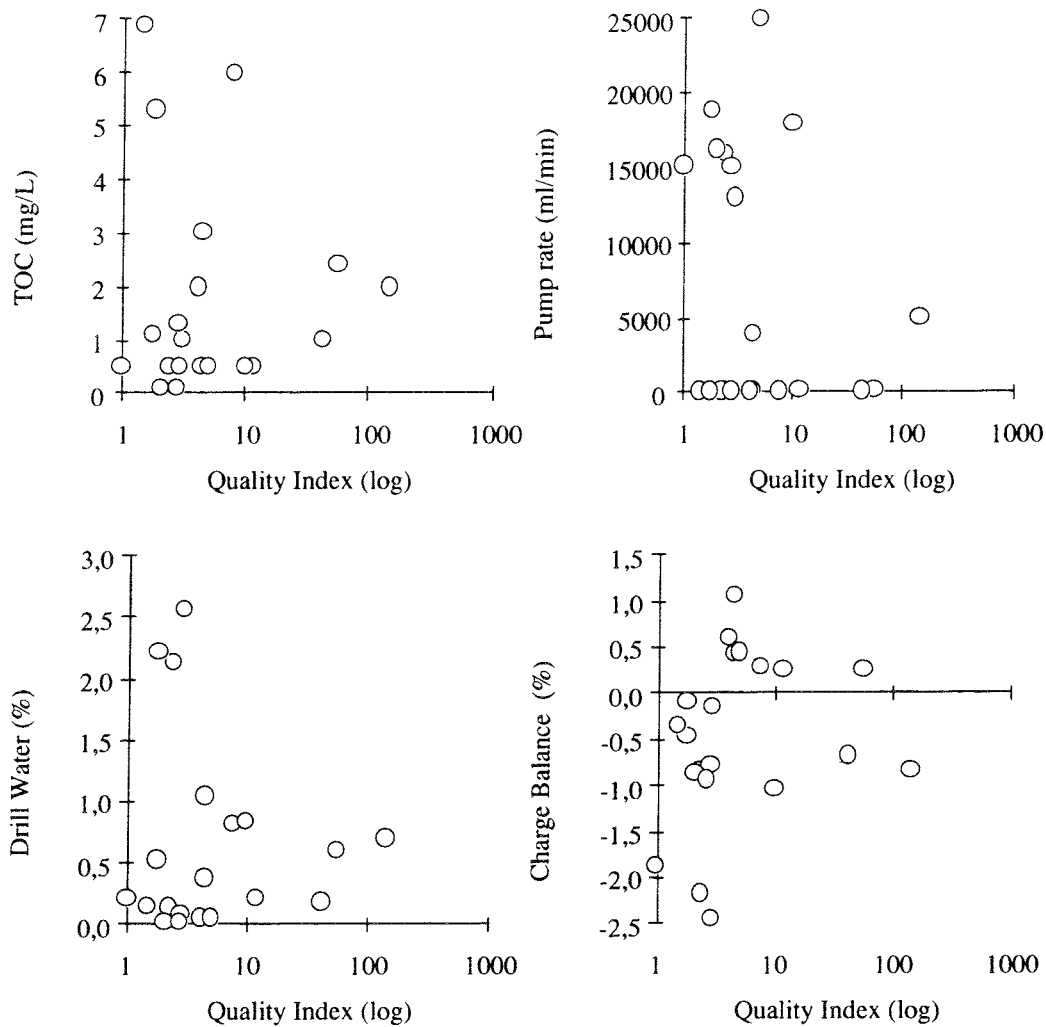


Figure 8. Total organic carbon, pump-rate, drilling water and charge balance are plotted against the quality index (high value = high quality).

For the quality index range shown in Figure 8, the method seems to indicate some correlation with the known quality indicating variables. In general, the plots show that the lower the TOC, drilling water, charge balance and pump extraction flow-rates are, the greater the chance of achieving some high quality groundwater samples. For other variables the correlation may be low and sometimes conflicting. The mixing calculations may also be insensitive to small disturbances which may have affected, for example, redox-sensitive elements, but not the main components used in the model. Another limitation with this method is the need to have several continuous groundwater samples collected from the same borehole section.

Perhaps one of the main advantages and use for this technique is to serve as a check as to whether the sampled section represents water which is either stagnant or is slowly moving through a bedrock of low hydraulic conductivity. Such samples, because of the low to very low conductivities, will tend to be shielded not only from natural dynamic groundwater mixing, but also from contaminating waters introduced during the drilling/testing activities etc.

A further application is estimating natural recharge/discharge conditions and/or assessing the effects of pumping in introducing formational groundwaters from shallower or deeper aquifers. This may be observed as mixing/dilution or mixing/concentration deviations in interconnected conductive fracture zones, where the former would indicate non-equilibrium recharge (shallower, fresh aquifer water) and the latter non-equilibrium discharge (deeper, saline aquifer water).

4 SPREADSHEET BASED QUALITY SCORING SYSTEM

4.1 Background

The aim was to create a powerful, reproducible yet simple and flexible quality scoring system to classify groundwater data. A standard spreadsheet program (Microsoft Excel 4.0) was used for this purpose. The objective was to formalise in a more mathematical way the often used variables and assumptions which form the basis of the manual classifications. The system is based on a simple quoting and scoring system. In order to test the method, data from all the Swedish and the Finnish sites at depth greater than 100 m, and containing ^2H and ^{18}O , were selected. From Sweden 75 observations from 23 deep (> 500 m) boreholes at 8 sites were considered; the Finnish data set contained 69 observations from 17 deep boreholes at 6 sites. The locations of the sites are shown in Figures 2 and 16, the data are listed in appendix 1.

4.2 Method

The starting point was to focus on the variables which may reflect disturbance of the downhole in situ conditions. The following 18 quality indicating variables were used; drilling water, pump-rate, oxygen, charge balance, time-lag of analyses, pH errors, Eh errors, distance between packers, tritium, partial pressure of carbon dioxide, ammonium, phosphate, total organic carbon, manganese, deuterium, oxygen-18, ferrous versus total iron ratio and sulphide.

Models were constructed to reflect the known or assumed general natural behaviour of these elements in the groundwater. The degree of deviation from the model is then calculated; the higher the deviation the lower the quality for that variable. The models check for possible known or assumed in situ, on-line, on-site or off-site errors. The relevance of the selected model for any specific data set is generally and easily checked using xy-plots. The models are often simple quotients which are easy to replace or modify based on later experience, special hydraulic conditions, or the number of special requirements for the data. Using such quotients the often arbitrary task to create relevant cut-off values are avoided since every result is on a continuous scale. There are three categories of models; quality-related, depth-related, and others (see Table 10).

The quality related models in Table 10 are mostly self explanatory, for example, the lower the drilling water content of the sample the higher the value and hence the quality. Special calculations for the charge balance are needed according to equation 1. The value is an absolute (ABS) value since exceeding a -10% or + 10% deviation is an indication of analytical discrepancies. The error between measured and calculated pH is based on the assumption that saturation index calculations of calcite should be close to zero. If not, the error is dependent on the measured pH (equation 3). It should be noted that no importance is given to whether the field value is an in-situ, on-line or off-site value. Instead this is represented by the time-lag of analyses; the quicker the analysis following sampling, the higher the scores (equation 2), although this is not always important, for example, cations to be analysed in samples preserved by acidification.

Table 10. Models used in the quality scoring system; the equations employed are explained in detail below.

Quality Related	Depth Related	Other
1 / Drilling water	Depth / ^3H	FeII / Fe(tot)
1 / Pump-rate	Depth / pCO_2	S^{2-}
1 / O_2	Depth / NH_4	
1 / Charge balance (Eq#1)	Depth / PO_4	
1 / Lag time of Analyses (Eq#2)	Depth / TOC	
1 / pH Error (Eq#3)	Mn / Depth	
1 / Eh Error (Eq#4, 5)	^2H / Depth	
1 / Distance between packers (Eq#6)	^{18}O / Depth	

Charge balance can be used as an indicator of the analytical quality of the analysis. The following equation was used (ABS = absolute value):

$$\text{Charge Balance} = \text{ABS } 100 \cdot \frac{(\text{cation equivalent / litre} - \text{anion equivalent / litre})}{(\text{cation equivalent / litre} + \text{anion equivalent / litre})} \quad \text{Eq\#1}$$

The lag time prior to the chemical analyses is calculated according to:

$$\text{Lag time of analyses: } < 6\text{h} = 6 \text{ or } > 6\text{h} = 24 \quad \text{Eq\#2}$$

The assumption is made that deep groundwater should be in equilibrium with the calcite. The deviation of the saturation index ($\log \text{IAP/KT}$) of calcite is caused by errors in the pH measurements according to:

$$\text{pH Error} = \text{ABS (SatIndex: Calcite)} \quad \text{Eq\#3}$$

Grenthe et al. (1992) have modelled all the Eh values measured within the SKB programme. The recorded values reflect equilibrium between the ferrous iron in solution and varying crystalline forms of ferric oxide ($\text{Fe}(\text{OH})_3$). Thus, using the $\text{Fe}_{(\text{II})}$ content in the groundwater and the measured pH, the measured Eh values can be corrected by using the following formula:

$$\text{Calculated (Eh)} = E_0^{\cdot} - (RT / F) (3\text{pH} + \log [\text{Fe}^{2+}]) \quad \text{Eq\#4}$$

$$\text{where } E_0^{\cdot} = 707 \text{ mV and } RT / F = 56\text{mV}$$

Where pH in this case is: measured pH - (Saturation Index of Calcite). The error between the measured Eh values and the calculated can then be evaluated by using the following formula:

$$\text{Eh Error} = \text{ABS (Measured Eh - Calculated Eh)} \quad \text{Eq\#5}$$

The larger the distance between the packers (Seclow = depth of the lower packer, Secup = depth of the upper packer) the increased risk of withdrawing foreign water according to:

$$\text{Distance Between Packers} = \text{Seclow} - \text{Secup} \quad \text{Eq\#6}$$

The error in the Eh measurements is based on a comparison between the calculated (Grenthe et al., 1992) and the measured value (equations 4 and 5); however, this approach is only valid when the groundwater Eh value is determined by the iron couple. Using equation 6 an increase in packer distance results in lower scores; this assumes that the risk to remove foreign water increases with increasing sampling borehole lengths.

In the depth-related model the results of the quotient calculations are relatively easy to explain. For example, high tritium found in deep bedrock sections give lower quality scores than the same amount of tritium in shallow sections. In general, this would be expected, although there are exceptions. Tritium, as a general indicator of shallow water conditions, is supported by calculating the high partial pressure of carbon dioxide using PHREEQE (Parkhurst et al., 1980). This has been used as an indication of shallow water (Laaksoharju, 1993) in combination with the other parameters in that category (e.g. TOC). Most of the redox-sensitive elements fall under the “other” model category.

These described models are simplifications that aim to describe the “undisturbed” in situ groundwater conditions. Therefore, as an example, the pH error calculations are valid in low conductive and moderate mixing situations. However, in fractures where different water types meet or in natural high mixing ratio zones, where supersaturation is obtained under natural conditions (Puidomènech and Nordstrom, 1987; Laaksoharju, 1990), the selected model would no longer be valid. In such a case the situation may instead be accounted for by the pump-rate quotient which may then reduce the scores.

The quotients are normalised to form weighted scores to avoid bias when small or large numbers are compared. The weighting is based on the number of observations in the data set. The more observations the higher the weight or importance for that specific variable. The higher the sum of the scores the higher the final quality score. The final quality score for the individual observation is expressed in percentages of the total scores of all observations. The working procedure and the Excel equations employed are shown in Figure 9.

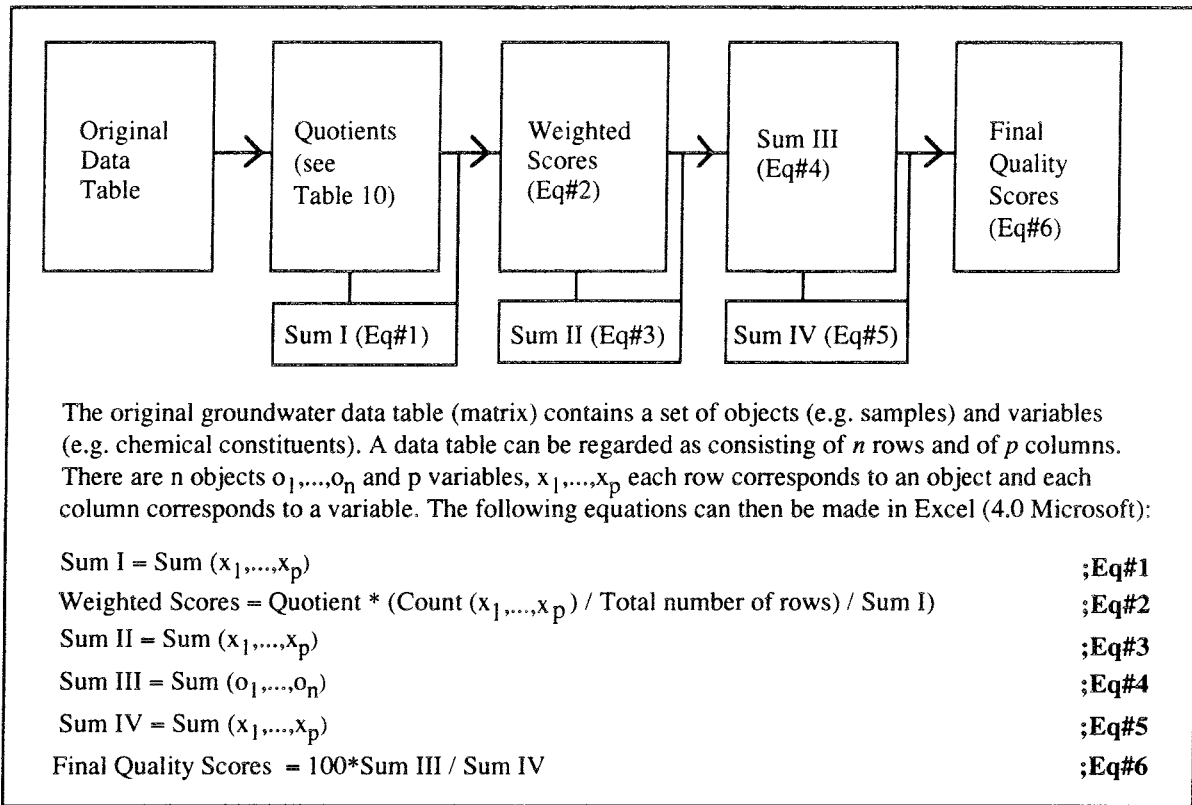


Figure 9. Working procedure; from the original value a quotient is calculated, the quotient is normalised to form weighted scores and Sum III summarises the final quality scores. The final quality scores are expressed in percentages of the total scores. Sum I and Sum IV are needed for the normalisation of the values and Sum II is needed when plotting the sum of the weighted scores for the individual variables.

4.3 Results

The calculated relative weights for the different variables in the quality scoring system is shown in Figure 10, and the average quality scores of the different models in the Swedish and Finnish data is shown in Figure 11. The average quality scores for the different sites in Sweden and Finland are illustrated as pie diagrams in Figures 12 - 14 (the numeric values are shown in Appendix 1). The summary pie diagram for the total scores in Finland and Sweden can be seen in Figure 15, and the location of the sites and the scores of the individual observations presented as xy-plots are illustrated in Figure 16.

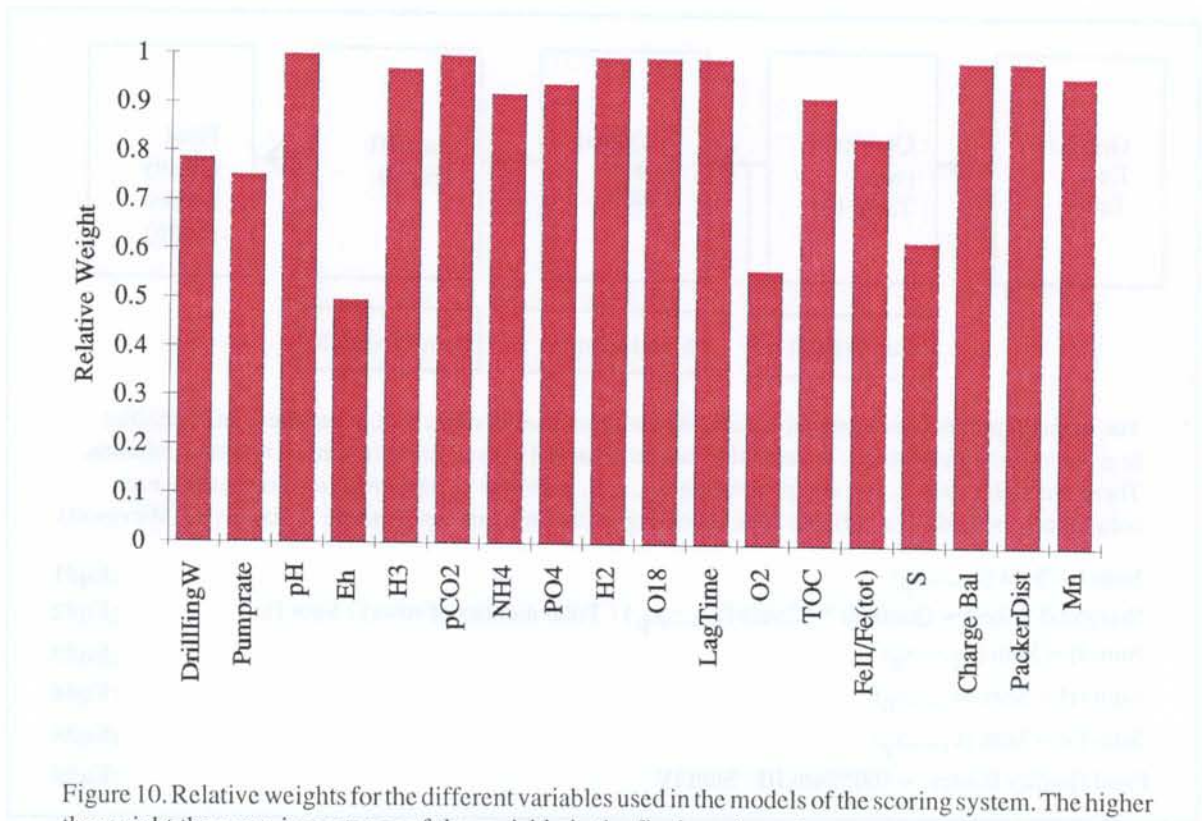


Figure 10. Relative weights for the different variables used in the models of the scoring system. The higher the weight the more importance of the variable in the final scoring scheme.

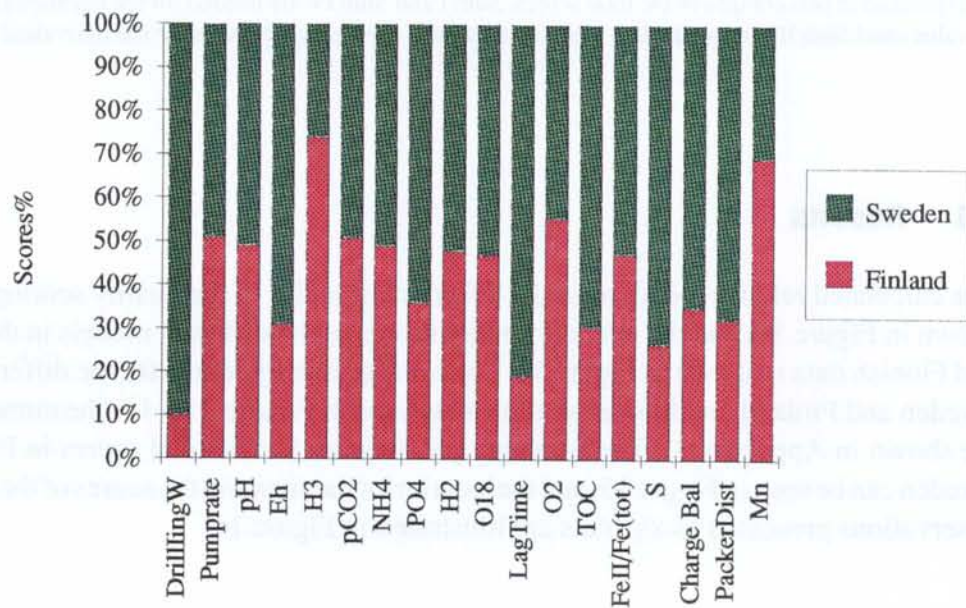


Figure 11. The gained quality scores (%) for the different measured parameters in the Swedish and Finnish groundwater data (the values add up to 100 percent). The higher the value the better the quality of the measured parameter.

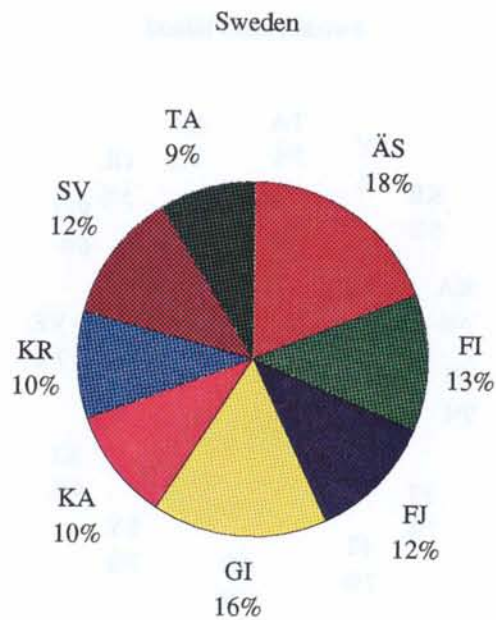


Figure 12. Average quality scores (%) for different sites in Sweden. The higher the score the better the quality of the sampled water at the site. (TA = Taavinunnanen, KA = Kamlunge, GI = Gideå, SV = Svartboberget, FI = Finnsjön, FJ = Fjällveden, ÄS = Äspö + Ävrö + Laxemar, KR = Kråkemåla).

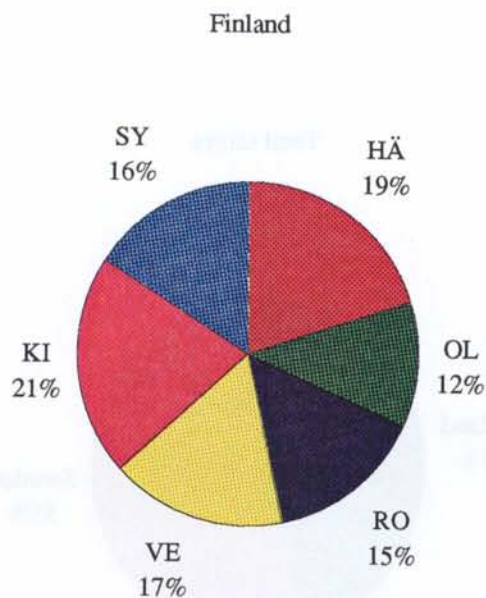


Figure 13. Average quality scores (%) for different sites in Finland. The higher the score the better the quality of the sampled water at the site. (OL = Olkiluoto, HÄ = Hästholmen, KI = Kivetty, SY = Syyry, RO = Romuvaara, VE = Veitsivaara).

Sweden and Finland

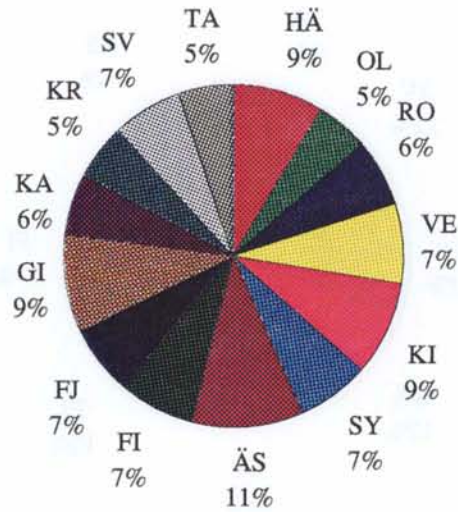


Figure 14. Average quality scores (%) comparing different sites in Sweden and Finland. The higher the scores the better the quality of the sampled water at the site. (Sweden: TA = Taavinunnanen, KA = Kamlunga, GI = Gideå, SV = Svartboberget, FI = Finnsjön, FJ = Fjällveden, S = Äspö + Ävrö + Laxemar, KR = Kråkemåla. Finland: OL = Olkiluoto, HÄ = Hästholmen, KI = Kivetty, SY = Syyry, RO = Romuvaara, VE = Veitsivaara).

Total scores

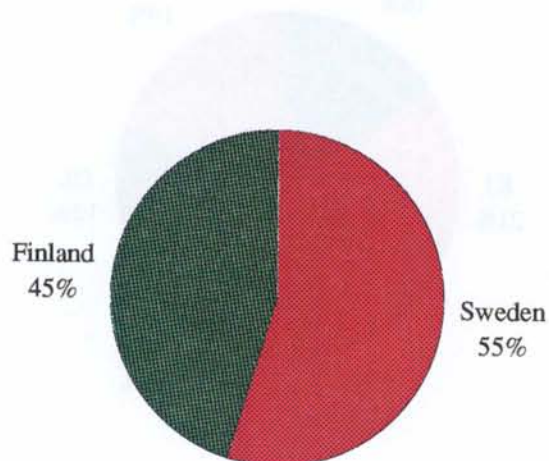


Figure 15. The total quality scores (%) of the Swedish and Finnish groundwater data. The higher the value the better the quality of the samples.

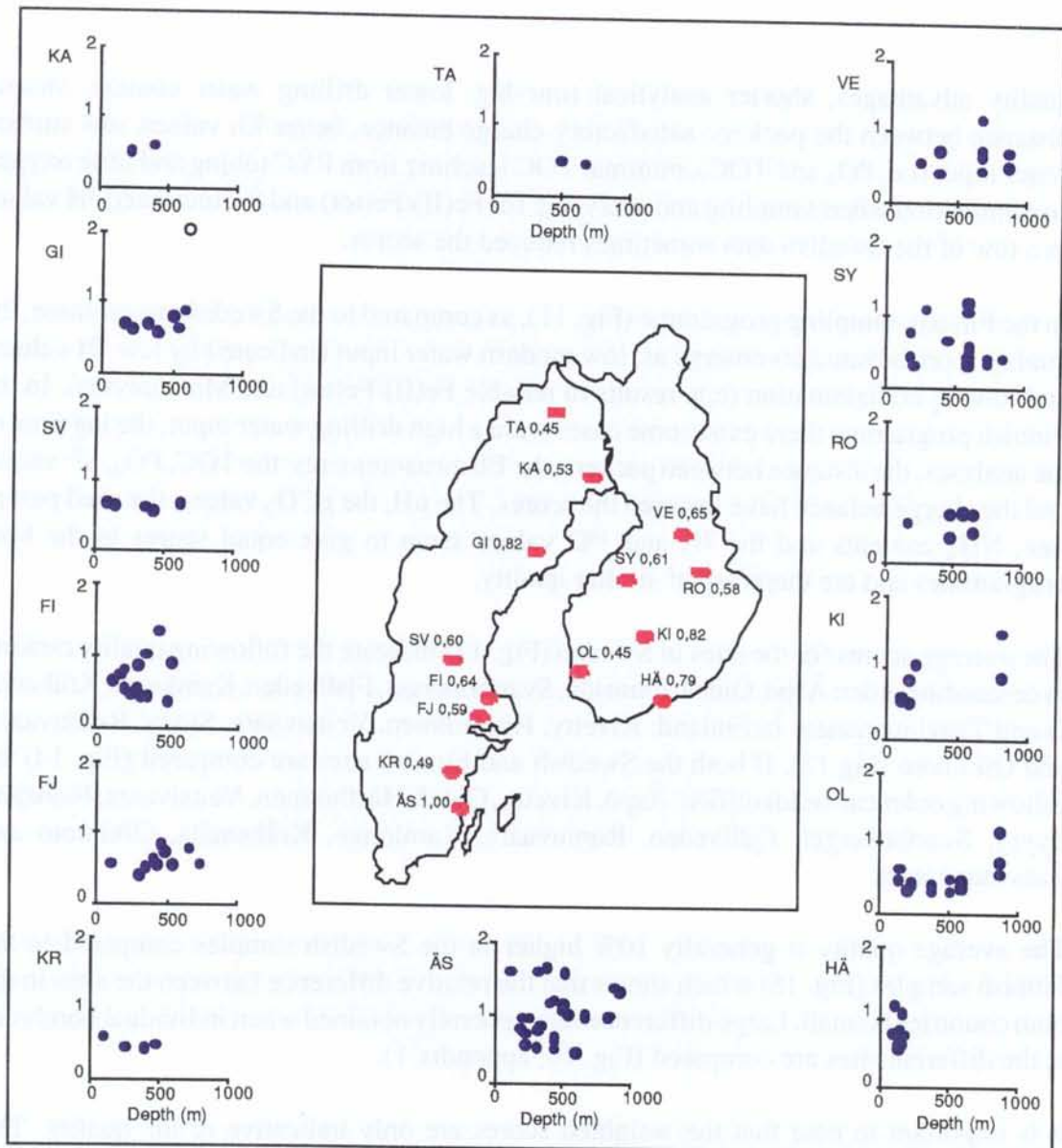


Figure 16. The map shows the average quality scores (%) from different sites in Sweden and Finland. The xy-plots show the scores (%) versus depth (m) for the observations at each site. The higher the scores the better the quality of the sampled water at the site. (Sweden: TA=Taavinunnanen, KA=Kamlunge, GI=Gideå, SV=Svartboberget, FI=Finnsjön, FJ=Fjällveden, KR=Kräkemåla, ÄS=Äspö+Ävrö+Laxemar. Finland: OL=Olkiluoto, HÄ=Hästholmen, KI=Kivetty, SY=Syry, RO=Romuvaara, VE=Veitsivaara).

4.4 Discussion

The relative weights for the different quotients (Fig. 10) are high (> 0.7) for most of the modelled data except for Eh error, O_s and S where the weighted score is about 0.5. Consequently, such models contribute about 50% of the cases to the final scores.

The quality scores for the different measured parameters (Fig. 11) indicate the Swedish sampling programme, compared to the Finnish programme, generally have the following

quality advantages; shorter analytical time-lag, lower drilling water content, shorter distance between the packers, satisfactory charge balance, better Eh values, low surface water input (i.e. PO_4 and TOC), minimal TOC leaching from PVC tubing and little oxygen contamination when sampling and analysing for Fe(II)/Fe(tot) and S^2 . Increased ^3H values in a few of the Swedish data sometimes reduced the scores.

In the Finnish sampling programme (Fig. 11), as compared to the Swedish programme, the quality score advantages emerge as; low modern water input (indicated by low ^3H values) and low O_2 contamination (e.g. results in reliable Fe(II)/Fe(tot) and Mn analyses). In the Finnish programme there exist some cases where a high drilling water input, the lag time of the analyses, the distance between packers, the Eh measurements, the TOC, PO_4 , S^{2-} values and the charge balance have lowered the scores. The pH, the pCO_2 values, the used pump-rate, NH_4 contents and the ^2H and ^{18}O values seem to give equal scores in the both programmes and are therefore of similar quality.

The average scores for the sites in Sweden (Fig. 12) indicate the following quality ranking in descending order: Äspö, Gideå, Finnsjön, Svartboberget, Fjällveden, Kamlunge, Kråkemåla and Taavinunnanen. In Finland: Kivetty, Hästholmen, Veitsivaara, Syyry, Romuvaara, and Olkiluoto (Fig. 13). If both the Swedish and Finnish sites are compared (Fig. 14) the following order can be identified: Äspö, Kivetty, Gideå, Hästholmen, Veitsivaara, Finnsjön, Syyry, Svartboberget, Fjällveden, Romuvaara, Kamlunge, Kråkemåla, Olkiluoto and Taavinunnanen.

The average quality is generally 10% higher in the Swedish samples compared to the Finnish samples (Fig. 15) which shows that the relative difference between the sites in the both countries is small. Large differences are generally obtained when individual boreholes at the different sites are compared (Fig. 16; appendix 1).

It is important to note that the weighted scores are only indicative of the quality. The selection of the sample population and the model employed may oversimplify or overemphasise the downhole in situ conditions. The difference in the quality scores of, for example, the pH measurements in Sweden and Finland, may be due to different flow conditions. Some of the Swedish sites are inland sites with relatively high natural groundwater circulation. The used pH correction model, which is appropriate in low flow conditions but inappropriate in mixing situations, may therefore lower the scores for some of the Swedish pH measurements. In addition, the difference in the Eh scores may in some cases be a result of the model employed which is based on the iron redox couple system (Grenthe et al., 1992). For example, in Olkiluoto the pyrite system is suggested to control the redox conditions in the upper part of the bedrock (Pitkänen et al., 1992a). The higher accuracy of the Swedish Eh measurements are often due to in situ downhole measurements; these facilities are not yet available for the Finnish programme. The differences in the analytical accuracy (charge balance) may reflect the greater number of on-site analyses carried out within the Swedish programme, but also the conducted pre-quality control of the dataset in GEOTAB.

In order to show the connection between the quality score calculations, based on many variables (18), and the individual variables, the final scores were plotted against the

following quality indicating variables; drilling water, pump-rate, charge balance, time-lag of analyses, ^3H and NH_4 (Fig. 17).

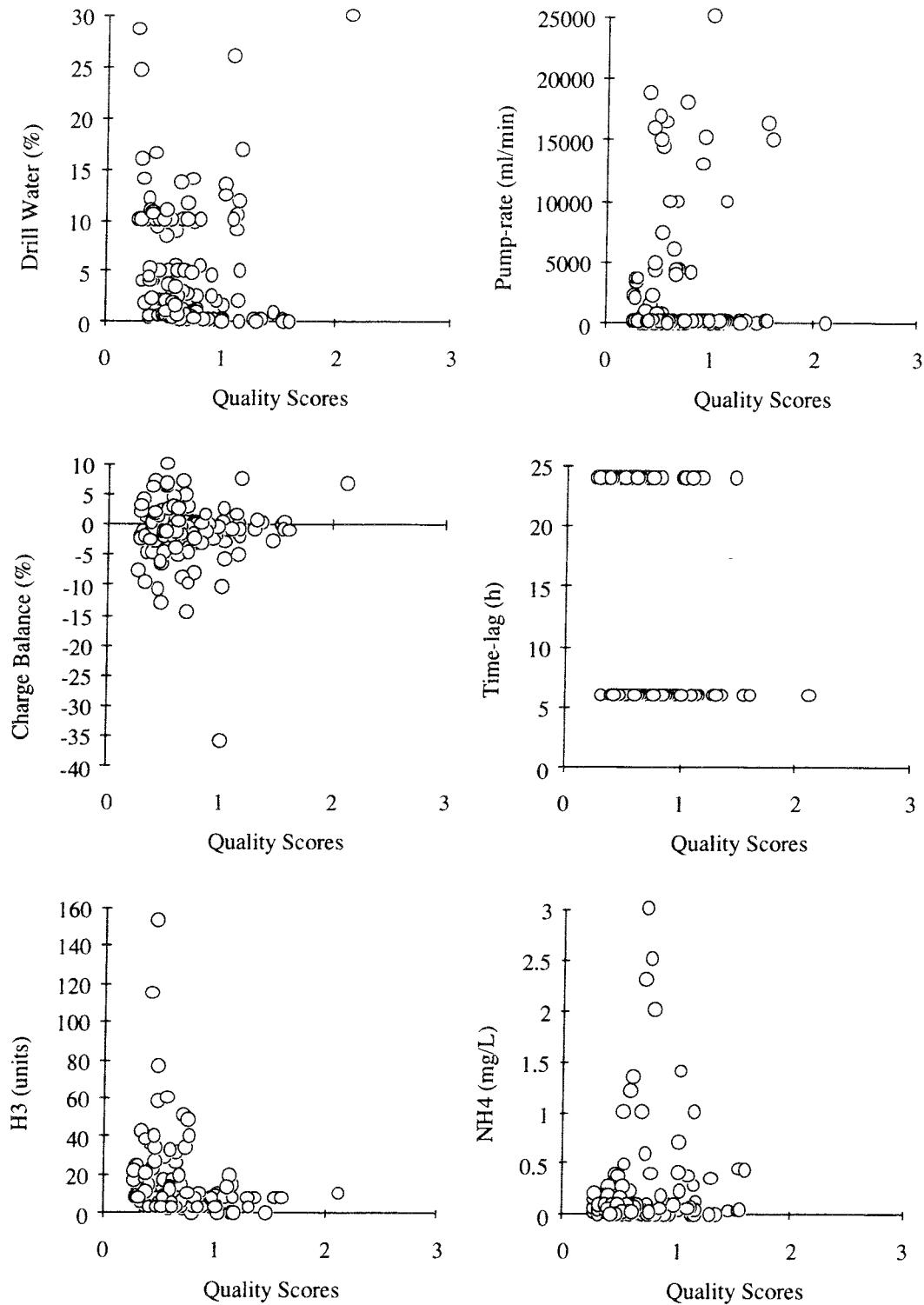


Figure 17. Drilling water, pump-rate, charge balance, analytical time-lag, ^3H and NH_4 are plotted against the quality scores for the SKB/TVO/IVO groundwaters. The higher the score the better the quality of the water.

Figure 17 indicates a variable correlation with these known quality indicating variables. The correlation is quite good with the charge balance, lag time of analyses, ^3H and NH_4 . Interestingly, for example, some high drilling water or pump-rate values have not lowered the scores dramatically, since the other 17 variables modelled simultaneously did not indicate any disturbance. Further cross-checking often indicated these values to be a single quality disturbance, not necessarily affecting the overall chemistry, and suggesting samples taken from a large, conductive, homogeneous aquifer.

Figure 18 shows a rather low correlation between quality and depth, and quality and distance from the coast. This is taken to indicate the independence of depth or location to the scoring system.

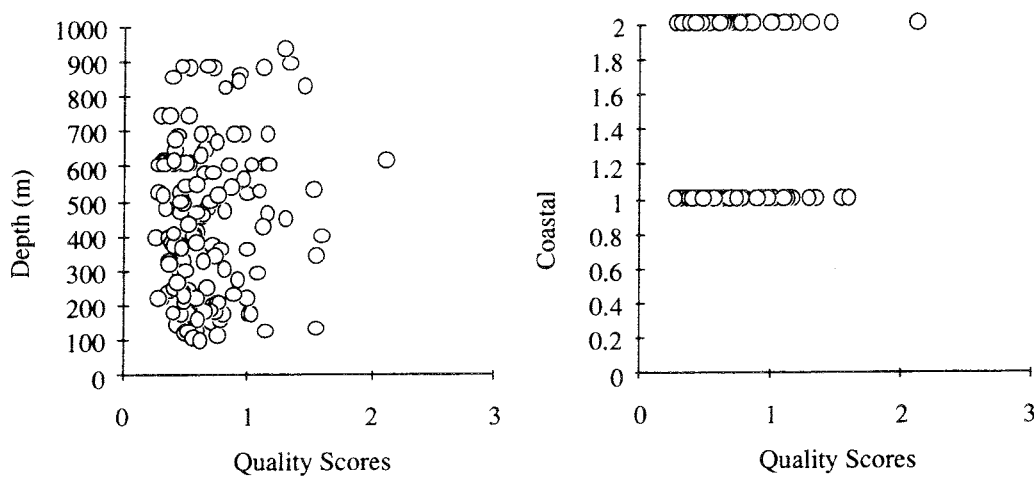


Figure 18. Quality scores related to bedrock depth and location (coastal = 1; inland = 2).

Summary

The scoring system has proven to be useful in judging objectively the quality of the groundwaters. With this approach many observations, representing both local and regional data, are scaled and sorted continuously. Most importantly, the calculations are easy to carry out and are reproducible. It is important to note that the models used are only preliminary, and new models may have to be constructed depending on the special requirements of a site or in the light of a particular problem. The basis of the scoring system will, however, remain unchanged. Any new or modified model can be easily integrated with the standard models.

One drawback is that the models applied may result in a strong simplification, underestimation or overestimation of the natural groundwater system being modelled. The results should therefore be treated as generalisations and need to be further interpreted using expert judgement.

5 EVALUATION AND DISCUSSION

High quality groundwater data are a necessary pre-requisite in site characterisation. For example, such data can provide useful information and understanding which may reduce conceptual uncertainties in bedrock models and groundwater flow simulations. Moreover, they serve as initial input parameters for site specific safety evaluation and can also provide quantitative or qualitative evidence of solute transport. The major aim of this study was to classify groundwaters from site investigation areas in Sweden and Finland based on quality, such that representative chemical compositions could be identified for further modelling purposes.

The question can be posed as to why quality evaluation of the data was necessary in the first place. This can be explained by the fact that both hydrogeochemical programmes have been undergoing continuous development since their inception. Inevitably mistakes have been made and it is only in recent years that a proper sampling and analytical protocol has been possible. The SKB and TVO site characterisation programmes to date have concentrated mainly in assessing the general quality of groundwater and understanding of the hydrogeochemical processes taking place in the bedrock. The presently demand for quality data is further increasing now that both the Swedish and Finnish programmes are being geared towards site-specific safety analysis during this decade.

In the past 10 years a considerable amount of data have been accumulated, and it has been the attempt through this present study to try and separate those data considered “representative” from data which should be treated with suspicion. Manual methods, based on experience and intimate knowledge of the sites, have been compared with mathematical and statistical methods, considered to be more objective, to try and establish a general protocol that could provide a qualitative and reliable groundwater database (present and future) for use in site evaluation and performance assessment. The risk to treat an observation containing new insights as an outlier is regarded as minimal since many interconnected variables are studied.

Different classification systems have been tested. These can be divided in two main separate groups; manual methods which are often sorting systems and computer based mathematical methods which are scoring systems. The early work on the SKB sites, and more recently at Äspö, describe the manual approach, these areas and those of the TVO programme have also been used to test the various mathematical models presented. The TVO sites represent an approach which has attempted to integrate mathematical objectivity (by using specific analytical cut-off limits) with manual interpretation. The ultimate goal was to describe how close the sampled waters reflect “undisturbed” in situ conditions in the bedrock.

Manual systems sort observations into useful and less useful categories, and are often based on quality-indicating parameters and calculations combined with experience of groundwater systems and logical judgement. This essentially means that a synthesis of water quality is based on establishing and understanding the interplay between many variables which can influence the quality of a sampled groundwater. This is achieved by being familiar with the analytical data and addressing all the potential sources which can influence the quality. A

certain amount of subjectivity is sometimes necessary to judge how important certain variables are, and to predict their consequences. The advantage is that qualitative information which may be difficult to express mathematically can be incorporated. The interrelationships between quantitative and qualitative data often prove to be decisive factors in groundwater quality evaluation. In addition, the manual treatment is flexible, site- or borehole-specific, and is also an essential part of the initial sorting and interpretation stage of the data.

Disadvantages may include the difficulty of reproducibility since some of the criteria cannot be quantitatively described, thus introducing a degree of subjectivity. Furthermore, different people may tend to emphasise different parameters of importance. The manual procedure may sometimes be too strict, for example, observations of lower quality are often not considered for further evaluation. It is also easy to set high standards of selection (i.e. tritium or no tritium; drilling water or no drilling water etc.) and there is a danger of being overly selective. In practice, however, as the overall judgement is based on the interplay of all influencing parameters, the emphasis of one parameter over the other tends to be minimised, and a balanced assessment generally results.

The mathematical models score observations on a continuous scale based on the response of selected quality indicating parameters. The less representative samples are not rejected but given a value indicating the confidence of the observation. Loss of information, effort and investment is hence minimised. Even though the selected models and assumptions are based on experience and logical judgement, which maybe somewhat subjective, they are strictly formulated so that reproducibility is reliable. The steps and models are well documented, which contrasts with the manual approach. The systems also handle many variables and a large amount of data with the same effort as using few observations. Furthermore, the models may be later modified and changed based on new data or site specific needs.

The main disadvantage is that the mathematical models tend to simultaneously oversimplify the system. Incomplete data sets for some variables may also lend bias to the results. There is also the danger that mathematical systems might become “blackboxes” which automatically process results reflecting the scientific limitations of the operator. The system is no better than the quality of the input data, the logical judgement used to formulate the parameters/criteria of importance and, ultimately, belief in the model.

The inability of directly comparing each of the quality evaluating approaches, due to the different methodologies and equipment used at the various sites and the wide variation of criteria used, prohibits an overall consensus of groundwater quality. The number of criteria common to each site is quite limited. For example, detailed hydraulic head measurements, i.e. required to calculate the water budget, one of the important criteria in establishing borehole contamination, are only available from some of the early SKB sites. In addition, the quality of the redox potential measurements, central to the SKB programme, has naturally meant that the SKB data are of a higher standard. On the other hand, the TVO programme has been more oriented towards collecting regional qualitative groundwater data to provide a comprehensive hydrogeochemical background on which to base the final

selection of their site-specific study areas. These sites are earmarked for more detailed hydrogeochemical studies in the future.

This heterogeneity of policy, methodology and techniques, is reflected in most of the classifications presented in this report which have found some credence within individual site-specific areas (i.e. the manual system), but have failed to adequately compare groundwater quality data between individual sites (since each site appears to be hydrogeologically unique) and also between the SKB and TVO hydrogeochemical programmes. The respective sites are geologically and hydraulically too complex, and the groundwater quality-influencing factors too numerous, to describe, quantify and compare.

Of the methods used, only the quality scoring system has managed to circumvent some of these problems by identifying and comparing mathematically chosen variables irrespective of the methodology or equipment used to measure them. However, only general comparisons can be made, any detailed interpretation of the data must rely on expert judgement. A method of quality evaluation to produce a suitable hydrogeochemical database for Sweden and Finland has been derived (appendix 1). As an illustration, the scoring method was used to compare the quality of the Swedish and Finnish data from 1984 to the present. This is demonstrated in Figure 19 which shows a general improvement in the Swedish data within this period. The Finnish data show variable degrees of improvement. The average quality is generally 10% higher in the Swedish samples compared to the Finnish samples. One explanation may be found in the different sampling methods used for example, the Finnish data from 1990-1992 are mainly derived from groundwaters collected during interference pump tests, which in many cases results in groundwater mixing and contamination. The results in Figure 19 also demonstrate the danger in judging the representativeness using the scoring method alone without the knowledge of the sampling conditions.

The different quality evaluation approaches used in this study have underlined several important points:

- * No one method is totally sufficient because of the complexity of the groundwater system.
- * It should always be borne in mind that an estimation of quality is at best only relative; in reality there are no "undisturbed" reference groundwaters available to evaluate the best classification system (such reference waters may be impossible to collect).
- * The manual testing system used in Finland, the statistical classification system and the system based on mixing need further development and testing to overcome their limitations.
- * The manual method used in Sweden is suggested as a natural starting point of the evaluation and exploration process when confronted with a new set of data.
- * The next step may be to introduce the scoring system for comparative purposes within and between the different site-specific areas.

- * There appear to be no reliable manual or mathematical short-cuts to evaluate groundwater quality; there is no substitute for artefact free sampling.

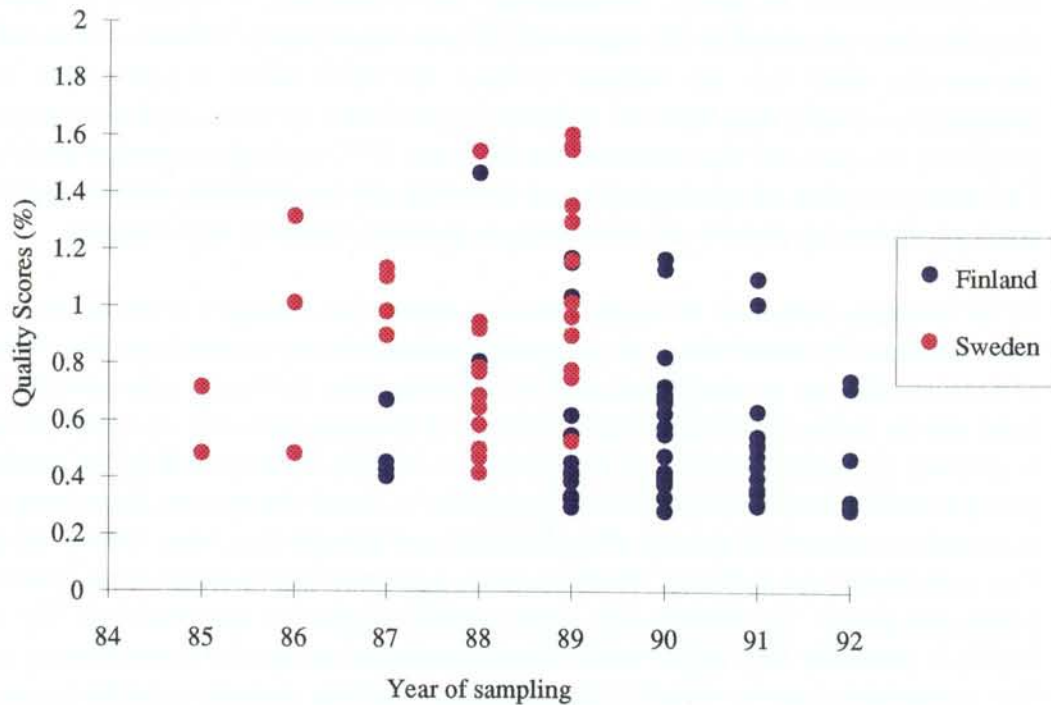


Figure 19. The groundwater quality scores versus the sampling year for the Swedish and Finnish data (SKB and TVO data).

Considering the future, since any groundwater quality evaluation and modelling of groundwater systems depend on high quality samples, resolving the issue of in situ, on-site and off-site errors must get first priority. Analytical accuracy may be improved to a certain degree, but most improvements may only be achieved by careful integration of *planning, co-ordination and close vigilance of field activities*. The best equipment and techniques available should be used. Therefore, if the quality of the field data can be ensured, then the need for the present “detective” work, using laborious evaluation methods or systems to identify the extent of groundwater contamination, should hopefully diminish.

6 ACKNOWLEDGEMENTS

This study was funded by SKB (Swedish Nuclear Fuel and Waste Management Co.), Sweden and TVO (Teollisuuden Voima Oy), Finland. We wish to thank Timo Äikäs, TVO and Peter Wikberg, SKB for their continuous support throughout and for the many discussions concerning the approach, planning and results of this co-operation project. The helpful comments from Fred Karlsson, SKB are gratefully acknowledged.

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8 APPENDIX

Data used in the modelling calculations including quality scores (%) for the individual boreholes. Swedish data are taken from the SKB data base GEOTAB and the Finnish data from TVO and IVO sources.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	QualityScores	IDCode	Depth(m)	Site	Year	pH(units)	Eh(mV)	Cl(mg/L)	Na(mg/L)	Ca(mg/L)	HCO3(mg/L)	SO4(mg/L)	Fe(mg/L)	FeII(mg/L)	Mn(mg/L)	PO4P(mg/L)	NH4N(mg/L)	S(mg/L)	TOC(mg/L)	ChargeBal%
2	0.61	H-Y1	176	HÄ	80	7.60	#N/A	5139	2040	780	65	610	1.040	#N/A	2.00	0.005	1.35	#N/A	3.2	-0.67
3	1.03	H-Y1	176	HÄ	82	7.50	#N/A	4759	1770	975	42	550	0.200	#N/A	1.80	0.010	0.70	#N/A	2.0	2.55
4	1.04	H-Y1	176	HÄ	83	7.60	#N/A	5070	2340	400	77	631	0.830	#N/A	1.80	0.010	1.40	#N/A	#N/A	-3.00
5	0.73	H-Y1	194	HÄ	85	7.60	#N/A	5245	2500	418	22	685	1.400	1.170	1.86	0.100	0.60	0.01	1.1	-2.58
6	1.16	H-Y1	124	HÄ	92	7.90	100	5000	2312	615	98	610	0.880	0.580	2.00	0.100	1.00	0.10	2.2	-0.07
7	0.73	H-Y2	147	HÄ	80	7.60	#N/A	5075	2250	580	93	638	0.700	#N/A	2.70	0.012	3.00	#N/A	2.0	-2.53
8	0.53	H-Y5	155	HÄ	81	8.00	#N/A	4276	1663	770	57	510	0.140	#N/A	1.60	0.090	1.00	#N/A	2.0	-1.71
9	0.60	H-Y5	155	HÄ	82	7.50	#N/A	5022	1870	910	70	680	0.600	#N/A	1.70	0.010	1.20	#N/A	2.0	-1.24
10	0.77	H-Y11	112	HÄ	82	7.70	#N/A	4317	1710	440	68	550	0.800	#N/A	2.00	0.010	2.50	#N/A	2.0	-7.98
11	0.80	H-Y11	160	HÄ	82	7.40	#N/A	5124	2250	540	81	660	1.200	#N/A	2.50	0.010	2.00	#N/A	2.0	-3.10
12	0.72	H-Y11	180	HÄ	82	7.40	#N/A	5126	2250	530	81	670	1.300	#N/A	2.40	0.010	2.30	#N/A	2.0	-3.90
13	0.45	OL-KR1	143	OL	89	8.10	-270	910	565	110	255	198	0.060	0.050	0.10	0.100	0.07	#N/A	2.0	-1.64
14	0.62	OL-KR1	163	OL	89	7.60	-5	1400	605	210	119	190	#N/A	#N/A	0.19	0.100	0.02	#N/A	#N/A	-5.24
15	0.33	OL-KR1	616	OL	90	8.80	-30	10000	3500	2700	21	0	0.360	0.300	0.33	0.100	0.06	0.05	11.0	1.42
16	0.42	OL-KR1	616	OL	90	8.90	-250	11500	3890	3100	13	0	0.380	0.300	0.38	0.100	0.04	0.05	6.9	0.51
17	0.40	OL-KR1	616	OL	90	8.90	-250	12000	4100	3300	13	0	0.380	0.300	0.39	0.100	0.04	0.05	5.9	1.32
18	0.72	OL-KR1	878	OL	90	8.50	35	20000	5688	5263	29	0	0.990	0.580	0.37	0.100	0.02	0.10	71.0	-4.65
19	1.14	OL-KR1	878	OL	90	8.80	-140	22000	6622	6214	27	0	0.380	0.020	0.40	0.100	0.01	0.10	44.0	-1.49
20	0.55	OL-KR1	878	OL	91	8.60	-10	13400	4621	3575	22	0	0.310	0.190	0.53	0.100	0.05	0.10	5.9	0.83
21	0.36	OL-KR1	607	OL	91	7.20	#N/A	759	450	107	271	110	2.500	2.500	0.12	0.017	0.09	#N/A	10.3	-1.26
22	0.44	OL-KR1	607	OL	91	7.70	#N/A	855	480	175	320	120	1.000	1.000	0.06	0.040	0.02	#N/A	14.7	0.25
23	0.31	OL-KR1	607	OL	91	7.60	#N/A	1582	720	445	315	123	0.510	0.500	0.13	0.030	0.06	#N/A	12.1	3.47
24	0.29	OL-KR1	525	OL	92	7.70	#N/A	2397	1010	500	259	104	1.000	1.000	0.24	0.019	0.07	#N/A	16.5	-1.91
25	0.47	OL-KR1	525	OL	92	7.80	#N/A	2045	960	428	293	105	1.500	1.500	0.18	0.002	0.39	#N/A	13.0	0.60
26	0.30	OL-KR1	220	OL	92	7.80	#N/A	508	390	82	329	128	0.420	0.420	0.12	0.071	0.02	#N/A	13.6	2.00
27	0.32	OL-KR1	220	OL	92	7.80	#N/A	421	360	74	347	118	0.250	0.250	0.10	0.120	0.01	#N/A	14.0	4.00
28	0.41	OL-KR2	238	OL	90	9.00	-50	555	386	77	303	104	0.300	0.230	0.14	0.100	0.09	0.05	11.2	-0.48
29	0.38	OL-KR2	238	OL	90	9.10	-160	570	386	77	297	108	0.230	0.160	0.14	0.420	0.09	0.05	11.6	-1.44
30	0.28	OL-KR3	391	OL	90	8.70	-70	2120	907	231	50	106	0.120	0.075	0.07	0.190	0.06	0.05	5.5	-7.77
31	0.38	OL-KR3	391	OL	90	8.60	-250	2600	1253	347	41	396	0.170	0.142	0.13	0.200	0.03	0.05	3.8	-3.66
32	0.43	RO-KR1	647	RO	87	6.90	-250	1	5	23	94	1	1.190	0.100	0.58	0.100	0.04	0.15	7.3	7.10
33	0.67	RO-KR1	647	RO	87	6.80	-330	1	4	21	87	1	0.960	0.300	0.62	0.100	0.02	0.05	6.6	6.97
34	0.55	RO-KR1	171	RO	89	7.00	#N/A	1	5	13	73	2	0.790	0.720	0.62	0.005	0.01	#N/A	1.0	-0.46
35	0.67	RO-KR1	580	RO	90	7.03	#N/A	1	6	12	92	2	1.000	0.970	0.81	0.002	0.01	#N/A	1.5	-9.02
36	0.72	RO-KR1	582	RO	90	7.28	#N/A	1	5	16	85	2	0.400	0.370	0.55	0.002	0.01	#N/A	1.1	0.79
37	0.68	RO-KR5	481	RO	90	9.05	-16	4	34	3	92	7	0.090	0.005	1.50	0.100	0.04	0.11	4.8	-1.47
38	0.35	RO-KR5	481	RO	91	9.25	230	7	34	3	91	5	0.029	0.004	0.00	0.200	0.05	0.09	4.6	-4.73
39	0.45	VE-KR1	688	VE	87	6.00	225	1	3	5	31	1	0.050	0.001	0.19	0.100	0.02	0.05	1.8	-10.65
40	0.40	VE-KR1	377	VE	87	6.10	260	1	3	4	25	1	0.050	0.001	0.18	0.100	0.02	0.05	1.0	-4.78
41	0.56	VE-KR1	233	VE	90	6.10	#N/A	1	5	9	40	1	0.280	0.120	0.56	0.002	0.01	#N/A	0.9	0.29
42	0.70	VE-KR1	691	VE	90	6.55	#N/A	2	7	18	64	7	0.750	0.750	0.40	0.003	0.01	#N/A	1.4	2.90
43	0.63	VE-KR1	691	VE	90	7.70	#N/A	8	20	18	81	4	0.300	0.190	0.07	0.004	0.01	#N/A	1.1	3.80
44	1.17	VE-KR1	691	VE	90	7.85	#N/A	12	24	17	93	4	0.030	0.170	0.00	0.002	0.01	#N/A	0.5	-1.95

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
QualityScores	IDCode	Depth(m)	Site	Year	pH(units)	Eh(mV)	Cl(mg/L)	Na(mg/L)	Ca(mg/L)	HCO3(mg/L)	SO4(mg/L)	Fe(mg/L)	FeII(mg/L)	Mn(mg/L)	PO4P(mg/L)	NH4N(mg/L)	S(mg/L)	TOC(mg/L)	ChargeBal%	
45	0.48	VE-KR1	883	VE	90	7.60	#N/A	15	22	18	74	3	0.890	0.300	0.12	0.005	0.02	#N/A	4.3	2.28
46	0.69	VE-KR1	883	VE	90	8.16	#N/A	19	28	17	81	1	0.160	0.010	0.02	0.002	0.02	#N/A	2.1	4.96
47	0.72	VE-KR4	370	VE	92	8.12	-86	5	11	17	91	3	0.290	0.220	0.04	0.100	0.01	0.01	4.1	-9.88
48	1.47	KI-KR1	825	KI	88	7.20	136	1	9	28	153	1	0.410	0.030	0.52	0.100	0.03	#N/A	30.0	-2.68
49	0.81	KI-KR1	175	KI	88	8.00	-300	1	10	22	122	0	0.080	0.080	0.18	0.100	0.03	0.07	5.8	-2.62
50	0.83	KI-KR1	822	KI	90	7.92	#N/A	6	27	19	128	1	0.900	0.470	0.20	0.009	0.03	#N/A	1.9	0.08
51	0.58	KI-KR1	119	KI	90	7.45	#N/A	2	12	33	146	2	0.250	0.220	0.60	0.002	0.01	#N/A	2.2	4.50
52	0.52	KI-KR1	119	KI	91	7.56	#N/A	1	12	32	140	2	0.100	0.070	0.52	0.005	0.01	#N/A	2.3	6.15
53	1.02	KI-KR2	220	KI	91	8.50	131	5	16	12	82	2	0.011	0.010	0.01	0.100	0.05	0.05	0.7	-10.28
54	0.48	KI-KR6B	175	KI	91	8.30	400	1	5	11	103	2	0.009	0.005	0.19	0.100	0.05	0.05	0.9	-6.70
55	0.32	SY-KR1	744	SY	89	9.10	-485	6650	1810	2100	26	0	0.060	0.040	0.00	0.100	0.05	0.05	6.8	-1.11
56	0.39	SY-KR1	744	SY	89	9.00	-487	6830	1870	2200	20	0	0.060	0.030	0.00	0.100	0.04	0.05	7.8	-0.40
57	1.16	SY-KR1	602	SY	89	7.80	-334	237	72	78	145	0	2.320	2.200	0.26	0.100	0.28	0.05	8.2	-4.91
58	0.41	SY-KR1	602	SY	89	8.30	-315	881	226	286	96	0	2.800	2.400	0.52	0.200	0.26	0.05	14.2	0.49
59	1.04	SY-KR1	602	SY	89	8.40	-308	2100	463	600	61	0	2.100	1.700	0.50	0.100	0.23	0.05	14.3	-5.96
60	0.30	SY-KR1	602	SY	89	8.40	-411	3405	823	1081	48	0	0.930	0.800	0.37	0.100	0.15	0.05	15.9	-2.35
61	1.18	SY-KR1	602	SY	89	8.30	-443	3460	1140	1260	35	0	0.380	0.350	0.24	0.100	0.12	0.10	6.4	7.40
62	0.34	SY-KR1	602	SY	89	8.50	-441	4285	1386	775	29	0	0.340	0.200	0.25	0.100	0.12	0.24	7.5	-9.61
63	0.42	SY-KR1	178	SY	89	8.60	-210	22	21	37	171	0	2.830	2.830	0.28	0.100	0.27	0.05	12.3	0.60
64	0.40	SY-KR1	855	SY	91	6.90	#N/A	5140	1650	1875	67	1	2.600	2.600	0.10	0.020	0.19	#N/A	3.2	6.14
65	0.55	SY-KR1	610	SY	91	7.02	#N/A	980	290	340	189	3	9.100	5.900	0.30	0.020	0.49	#N/A	6.1	0.64
66	0.51	SY-KR1	610	SY	91	7.32	#N/A	1540	410	430	134	2	7.200	7.000	0.62	0.010	0.01	#N/A	5.8	-4.89
67	0.30	SY-KR1	220	SY	91	6.50	#N/A	4	19	26	153	1	2.700	2.600	0.20	0.040	0.21	#N/A	5.4	3.18
68	0.64	SY-KR2	455	SY	91	8.33	-37	830	354	180	107	20	0.120	0.020	0.07	0.100	0.08	0.08	2.0	-0.74
69	1.10	SY-KR6	292	SY	91	9.02	-174	1338	540	287	34	10	0.021	0.001	0.01	0.100	0.37	1.30	1.1	-0.72
70	0.75	SY-KR6	181	SY	92	9.25	-181	1060	460	215	28	11	0.025	0.019	0.00	0.100	0.01	0.77	2.6	0.43
71	0.93	KLX01	275	AS	88	8.48	-241	2050	1040	243	83	48	0.129	0.129	0.20	0.001	0.08	0.53	1.5	-0.39
72	0.65	KLX01	459	AS	88	8.20	#N/A	1700	860	223	78	106	0.041	0.040	0.16	0.003	0.06	0.46	1.4	-1.35
73	0.97	KLX01	691	AS	89	7.60	#N/A	4680	1610	1330	24	390	0.135	0.135	0.21	0.003	0.04	0.65	3.3	-0.68
74	0.78	KAS02	208	AS	89	7.40	#N/A	3820	1300	990	71	106	0.502	0.483	0.91	0.010	0.40	0.50	6.0	0.24
75	0.50	KAS02	326	AS	88	7.61	-152	5360	1710	1480	33	291	0.719	0.624	0.67	0.010	0.37	0.15	2.0	-0.94
76	0.59	KAS02	466	AS	88	8.33	-213	5440	1800	1580	25	290	0.964	0.941	0.73	#N/A	0.22	0.13	3.0	0.98
77	1.55	KAS02	533	AS	88	8.00	-311	6330	2200	1890	10	550	0.244	0.240	#N/A	0.003	0.03	0.18	#N/A	-0.21
78	0.95	KAS02	863	AS	88	8.16	-5	11100	2850	3690	7	522	0.027	0.023	0.19	0.010	0.01	0.01	0.5	-2.01
79	1.36	KAS02	892	AS	89	8.55	-164	11100	3000	3830	11	519	0.051	0.049	0.23	0.020	0.01	0.72	0.5	0.12
80	1.57	KAS03	132	AS	89	7.98	-284	1220	613	162	61	31	0.125	0.123	0.10	0.001	0.04	0.71	2.0	0.53
81	0.77	KAS03	209	AS	88	7.66	-96	2850	1200	472	54	#N/A	#N/A	#N/A	0.39	0.003	#N/A	0.05	1.0	-0.12
82	0.69	KAS03	250	AS	88	7.80	-128	2950	1290	490	53	39	#N/A	#N/A	0.35	0.003	#N/A	0.15	0.5	0.31
83	0.79	KAS03	360	AS	88	7.80	#N/A	5180	1770	1400	12	370	#N/A	#N/A	0.27	0.001	#N/A	0.05	0.5	-1.16
84	0.47	KAS03	467	AS	88	7.78	-104	4600	1550	1190	27	300	#N/A	#N/A	0.27	#N/A	#N/A	0.11	0.5	-2.26
85	0.42	KAS03	616	AS	88	8.07	-68	5880	1920	1740	11	470	#N/A	#N/A	0.24	#N/A	#N/A	0.05	1.1	-0.63
86	0.93	KAS03	846	AS	88	8.04	-79	8080	2130	2670	11	680	0.053	0.047	0.23	0.002	#N/A	0.11	0.5	-2.58
87	1.30	KAS03	931	AS	89	7.28	-270	12300	3020	4380	11	709	0.078	0.077	0.20	#N/A	0.01	1.28	#N/A	-0.99

I	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	QualityScores	IDCode	Depth(m)	Site	Year	pH(units)	Eh(mV)	Cl(mg/L)	Na(mg/L)	Ca(mg/L)	HCO3(mg/L)	SO4(mg/L)	Fe(mg/L)	FeII(mg/L)	Mn(mg/L)	PO4P(mg/L)	NH4N(mg/L)	S(mg/L)	TOC(mg/L)	ChargeBal%
88	0.90	KAS04	231	AS	89	7.76	-302	508	382	91	222	180	0.041	0.040	#N/A	0.008	0.01	1.10	6.9	-0.43
89	0.75	KAS04	339	AS	89	7.90	-286	3030	1180	740	69	220	0.327	0.324	0.31	0.003	0.09	0.41	5.3	-0.19
90	1.17	KAS04	460	AS	89	8.06	-288	5840	1890	1660	21	407	0.259	0.256	0.44	0.001	0.05	0.60	1.3	-0.87
91	0.53	KAS06	241	AS	89	7.60	#N/A	3630	1230	893	89	150	0.442	0.440	0.68	0.003	0.27	0.17	4.7	-0.88
92	1.56	KAS06	341	AS	89	7.50	#N/A	5680	1820	1490	49	283	0.431	0.425	0.83	0.005	0.44	0.02	0.1	-0.96
93	1.61	KAS06	398	AS	89	7.50	#N/A	5970	2070	1410	64	362	0.848	#N/A	1.11	0.005	0.42	0.01	0.1	-1.01
94	1.02	KAS06	521	AS	89	7.50	#N/A	6150	2200	1570	50	459	0.631	0.627	0.88	0.004	0.41	0.02	0.5	0.35
95	1.14	KAV01	423	AS	87	7.36	-218	575	255	156	186	43	1.690	1.680	3.00	0.001	0.07	0.63	9.6	1.58
96	1.11	KAV01	527	AS	87	6.92	-288	1970	750	440	81	118	2.230	2.230	2.40	0.005	0.06	1.20	#N/A	-0.97
97	0.98	KAV01	561	AS	87	7.19	-277	4300	1500	1100	42	220	1.020	1.020	1.70	0.010	0.08	0.81	#N/A	-0.66
98	0.90	KAV01	689	AS	87	6.50	-130	9700	3100	2900	9	400	#N/A	#N/A	0.18	0.003	#N/A	0.01	0.5	-0.13
99	0.48	BFI01	289	FI	86	6.79	373	5200	1700	1500	59	370	0.022	0.009	1.10	0.005	#N/A	0.01	#N/A	1.08
100	1.01	BFI01	360	FI	86	7.36	345	5300	#N/A	1500	59	400	#N/A	#N/A	1.00	0.002	#N/A	0.01	#N/A	-36.01
101	1.32	BFI01	449	FI	86	7.04	295	5500	1700	1650	47	370	0.016	0.005	0.82	0.005	0.35	0.01	18.0	0.63
102	0.78	KFI01	209	FI	80	7.60	#N/A	11	45	61	320	1	19.000	18.000	0.33	0.040	0.02	#N/A	11.0	0.08
103	0.46	KFI01	296	FI	80	7.60	#N/A	37	88	50	350	1	21.000	20.000	0.29	0.080	0.05	#N/A	9.8	0.44
104	0.43	KFI04	250	FI	80	7.80	#N/A	74	170	24	390	30	6.100	6.100	0.08	0.050	0.16	#N/A	10.0	-1.20
105	0.42	KFI04	371	FI	80	7.80	#N/A	72	165	22	395	29	9.700	7.800	0.08	0.030	0.18	#N/A	7.8	-3.00
106	0.87	KFI04	537	FI	80	7.70	#N/A	75	170	22	393	19	7.900	2.400	0.05	0.030	0.17	#N/A	7.8	-1.16
107	0.50	KFI05	208	FI	80	7.30	#N/A	3450	1100	900	83	325	6.200	3.400	0.67	0.040	0.02	#N/A	3.6	-1.64
108	0.51	KFI05	300	FI	80	7.40	#N/A	4650	1380	1500	39	300	2.400	2.400	0.47	0.050	0.16	#N/A	1.9	0.96
109	0.61	KFI07	126	FI	80	7.80	#N/A	23	94	36	333	7	2.900	2.900	0.13	0.010	0.05	#N/A	6.2	0.17
110	0.83	KFI07	304	FI	80	8.30	#N/A	665	390	114	233	71	0.570	0.530	0.06	0.010	0.02	#N/A	4.4	0.07
111	0.39	KFI07	325	FI	80	8.20	#N/A	380	224	107	292	35	5.200	4.100	0.12	0.020	0.03	#N/A	6.0	0.34
112	0.33	KFI07	514	FI	80	8.10	#N/A	555	275	142	278	49	7.000	1.800	0.13	0.040	0.09	#N/A	5.7	-1.93
113	0.71	KFI09	185	FI	85	7.40	-271	2800	950	370	162	210	1.090	1.070	0.84	0.002	1	0.44	7.5	-14.69
114	0.48	KFI09	363	FJ	85	7.66	-412	5100	1400	1000	33	300	0.350	0.340	#N/A	0.003	#N/A	0.01	#N/A	-13.23
115	0.54	KFJ02	124	FJ	82	7.70	#N/A	5	37	18	160	6	1.100	0.950	0.18	0.015	0.07	0.06	5.0	-1.77
116	0.38	KFJ04	318	FJ	82	7.50	#N/A	9	38	28	196	7	10.000	8.100	0.30	0.015	0.09	0.01	7.0	-2.58
117	0.61	KFJ04	411	FJ	82	8.45	-99	5	54	17	195	4	1.400	1.370	0.09	0.034	0.07	0.04	6.0	-0.14
118	0.71	KFJ04	497	FJ	82	8.40	-166	8	62	14	198	4	1.400	1.200	0.09	0.020	0.04	0.13	8.0	-0.33
119	0.53	KFJ07	433	FJ	83	8.57	-127	1	47	11	150	1	1.000	1.000	0.06	#N/A	0.03	0.01	11.0	6.56
120	0.52	KFJ07	543	FJ	83	7.31	-182	3	53	11	150	1	0.590	0.470	0.08	#N/A	0.02	0.01	18.0	9.90
121	0.54	KFJ07	741	FJ	83	7.56	-409	4	52	11	190	1	0.090	0.050	0.06	#N/A	0.01	0.01	13.0	-2.91
122	0.83	KFJ08	471	FJ	82	8.55	-119	4	13	25	130	7	2.900	2.200	0.15	0.008	0.01	0.01	3.0	-3.24
123	0.76	KFJ08	667	FJ	82	8.92	-184	4	14	26	130	5	3.200	2.700	0.15	0.016	0.01	0.01	3.0	-1.65
124	0.66	KGI02	179	GI	82	8.50	#N/A	4	48	10	161	1	0.180	0.180	0.01	0.010	0.08	0.01	4.0	-0.53
125	0.65	KGI02	329	GI	82	8.80	-61	5	49	10	163	1	0.590	0.590	0.02	0.003	0.06	0.03	5.0	-1.75
126	0.58	KGI02	401	GI	82	8.62	-49	5	53	10	160	0	0.590	0.410	0.02	0.008	0.06	0.04	3.0	2.27
127	0.60	KGI02	545	GI	82	8.82	-95	5	51	10	160	0	0.820	0.780	0.02	0.008	0.05	0.02	3.0	0.63
128	0.86	KGI02	603	GI	82	8.66	-89	5	50	11	158	0	0.650	0.600	0.03	0.021	0.05	0.03	2.0	1.59
129	0.59	KGI04	223	GI	82	8.99	-71	8	49	9	133	0	0.240	0.130	0.01	0.011	0.01	0.04	5.0	-0.71
130	0.54	KGI04	405	GI	82	9.33	-13	178	105	21	18	0	0.070	0.050	0.01	0.008	0.01	0.01	2.0	2.38

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	QualityScores	IDCode	Depth(m)	Site	Year	pH(units)	Eh(mV)	Cl(mg/L)	Na(mg/L)	Ca(mg/L)	HCO3(mg/L)	SO4(mg/L)	Fe(mg/L)	FeII(mg/L)	Mn(mg/L)	PO4P(mg/L)	NH4N(mg/L)	S(mg/L)	TOC(mg/L)	ChargeBal%
131	0.77	KGI04	513	GI	82	8.22	-77	2	5	30	121	8	8.500	7.300	0.28	0.008	0.01	0.01	2.0	-2.53
132	2.13	KGI04	617	GI	82	7.84	-295	260	145	58	50	0	5.400	#N/A	0.19	#N/A	#N/A	#N/A	#N/A	6.68
133	0.50	KKA03	233	KA	79	6.30	#N/A	20	17	127	265	160	27.000	26.000	1.05	0.042	0.08	#N/A	23.0	-1.85
134	0.50	KKA04	227	KA	80	7.30	#N/A	37	53	75	293	118	10.000	2.300	0.54	0.075	0.06	#N/A	4.6	-4.58
135	0.58	KKA04	398	KA	80	7.30	#N/A	41	58	80	295	112	14.000	1.100	0.56	0.110	0.05	#N/A	4.6	-2.23
136	0.58	KKR01	104	KR	78	7.30	#N/A	15	40	40	224	4	4.800	#N/A	0.42	0.003	0.09	#N/A	5.2	2.86
137	0.45	KKR01	265	KR	78	7.90	#N/A	23	57	28	227	2	2.500	#N/A	#N/A	0.007	0.10	#N/A	4.0	1.13
138	0.42	KKR01	407	KR	78	8.10	#N/A	280	250	29	215	39	3.500	#N/A	0.06	0.020	0.06	#N/A	2.6	1.81
139	0.49	KKR01	492	KR	78	7.80	#N/A	47	82	21	222	8	5.300	#N/A	0.22	0.010	0.09	#N/A	3.9	-1.15
140	0.63	KSV04	97	SV	82	8.20	#N/A	2	24	25	138	2	0.220	0.040	0.05	0.002	0.02	0.01	3.0	2.36
141	0.60	KSV04	377	SV	82	7.16	-142	9	40	13	127	1	0.490	0.210	0.03	0.134	0.02	0.03	12.0	-1.36
142	0.53	KSV04	431	SV	82	9.05	-75	8	35	17	130	1	0.690	0.250	0.05	0.023	0.02	0.01	3.0	-1.29
143	0.63	KSV04	631	SV	82	8.70	#N/A	7	35	17	126	1	0.440	0.270	0.04	0.026	0.02	0.01	4.0	0.42
144	0.61	KSV05	161	SV	82	5.87	115	2	20	19	114	3	1.800	1.800	0.07	0.002	0.02	0.02	2.0	-3.86
145	0.47	KTA01	497	TA	83	8.40	#N/A	1	4	6	31	7	0.970	0.010	0.02	0.010	0.01	0.01	4.7	-6.32
146	0.43	KTA01	677	TA	83	9.46	360	1	5	7	30	6	1.400	0.260	0.01	0.030	0.01	0.01	12.0	1.96

	A	B	C	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
1	QualityScores	IDCode	Depth(m)	H3(units)	D(prom)	O18(prom)	O2(mg/L)	DrillWater(%)	PumpRate(ml/min)	LagTime(h)	Log pCO2	Log Calcite(SI)	pH(Calc)	Eh(Calc)	PackerDist(m)	Coastal
2	0.61	H-Y1	176	7	-67.8	-8.5	#N/A	8.80	#N/A	24	-3.02	0.21	7.4	#N/A	3	1
3	1.03	H-Y1	176	1	-70.9	-9.1	#N/A	1.60	#N/A	24	-3.11	0.02	7.5	#N/A	4	1
4	1.04	H-Y1	176	10	-64.7	-8.3	#N/A	13.50	#N/A	24	-2.92	0.01	7.6	#N/A	4	1
5	0.73	H-Y1	194	2	-66.0	-7.8	0.02	2.20	60	24	-3.47	-0.52	8.1	-395	4	1
6	1.16	H-Y1	124	8	-61.6	-7.9	0.60	2.00	60	24	-3.13	0.60	7.3	-241	3	1
7	0.73	H-Y2	147	3	-63.1	-8.0	#N/A	#N/A	#N/A	24	-2.85	0.25	7.3	#N/A	4	1
8	0.53	H-Y5	155	6	-71.7	-9.1	#N/A	8.50	#N/A	24	-3.45	0.59	7.4	#N/A	4	1
9	0.60	H-Y5	155	2	-66.9	-8.6	#N/A	2.70	#N/A	24	-2.89	0.20	7.3	#N/A	4	1
10	0.77	H-Y11	112	7	-67.4	-8.9	#N/A	9.73	#N/A	24	-3.06	0.14	7.6	#N/A	4	1
11	0.80	H-Y11	160	2	-63.3	-8.1	#N/A	2.60	#N/A	24	-2.71	-0.05	7.4	#N/A	4	1
12	0.72	H-Y11	180	2	-63.2	-8.2	#N/A	2.70	#N/A	24	-2.71	-0.06	7.5	#N/A	4	1
13	0.45	OL-KR1	143	#N/A	-85.2	-9.9	0.17	9.40	130	24	-3.11	0.40	7.7	-248	5	1
14	0.62	OL-KR1	163	7	-91.9	-10.1	0.08	5.50	8	24	-2.67	0.14	7.5	#N/A	5	1
15	0.33	OL-KR1	616	11	-69.5	-9.1	0.37	4.00	100	24	-4.89	1.23	7.6	-270	5	1
16	0.42	OL-KR1	616	8	-64.4	-8.7	0.18	4.00	80	24	-5.28	1.18	7.7	-295	5	1
17	0.40	OL-KR1	616	8	-64.4	-8.7	0.10	4.00	80	24	-5.27	1.13	7.8	-304	5	1
18	0.72	OL-KR1	878	#N/A	-65.8	-9.2	4.68	11.60	4	24	-4.47	1.30	7.2	-223	247	1
19	1.14	OL-KR1	878	8	-70.3	-9.0	-0.20	10.40	3	24	-4.93	1.51	7.3	-156	247	1
20	0.55	OL-KR1	878	9	-73.3	-10.4	0.02	4.80	20	24	-4.67	1.16	7.4	-237	247	1
21	0.36	OL-KR1	607	17	-87.2	-10.7	0.00	10.00	550	24	-1.93	-0.16	7.4	-286	30	1
22	0.44	OL-KR1	607	17	-86.5	-10.7	0.00	10.00	1450	24	-2.33	0.63	7.1	-215	30	1
23	0.31	OL-KR1	607	17	-86.2	-10.8	0.10	10.00	3440	24	-2.27	0.84	6.8	-145	30	1
24	0.29	OL-KR1	525	17	-76.7	-10.6	0.30	10.00	2220	24	-2.46	0.88	6.8	-173	31	1
25	0.47	OL-KR1	525	17	-84.3	-10.7	0.30	10.00	2220	24	-2.50	0.98	6.8	-182	31	1
26	0.30	OL-KR1	220	25	-84.5	-10.7	0.80	10.00	3640	24	-2.40	0.46	7.3	-239	359	1
27	0.32	OL-KR1	220	25	-82.0	-11.0	0.90	10.00	3640	24	-2.37	0.45	7.4	-229	359	1
28	0.41	OL-KR2	238	21	-84.7	-10.8	0.43	0.60	80	24	-3.66	1.53	7.5	-246	5	1
29	0.38	OL-KR2	238	18	-85.7	-10.8	#N/A	0.40	75	24	-3.78	1.61	7.5	-241	5	1
30	0.28	OL-KR3	391	22	-83.8	-9.8	0.93	28.60	120	24	-4.18	0.86	7.8	-281	5	1
31	0.38	OL-KR3	391	8	-91.3	-11.1	-0.18	12.00	150	24	-4.18	0.78	7.8	-294	5	1
32	0.43	RO-KR1	647	36	-101.5	-13.1	0.05	16.50	82	24	-2.10	-1.39	8.3	-363	5	2
33	0.67	RO-KR1	647	26	-100.5	-13.2	0.01	3.00	82	24	-2.06	-1.58	8.4	-405	5	2
34	0.55	RO-KR1	171	29	-110.1	-13.1	0.20	10.00	7350	24	-2.28	-1.61	8.6	-465	30	2
35	0.67	RO-KR1	580	32	-101.8	-13.1	0.90	10.00	6050	24	-2.21	-1.51	8.5	-462	788	2
36	0.72	RO-KR1	582	10	-102.3	-13.2	0.50	10.00	4290	24	-2.45	-1.14	8.4	-417	785	2
37	0.68	RO-KR5	481	10	-103.7	-13.5	0.01	3.00	43	24	-4.16	-0.11	9.2	-437	42	2
38	0.35	RO-KR5	481	43	-103.1	-13.7	0.08	1.78	33	24	-4.25	0.17	9.1	-418	42	2
39	0.45	VE-KR1	688	23	-104.0	-13.6	5.50	0.60	80	24	-2.10	-3.79	9.8	-496	5	2
40	0.40	VE-KR1	377	38	-102.4	-13.7	6.50	0.60	78	24	-2.22	-3.79	9.9	-512	5	2
41	0.56	VE-KR1	233	17	-97.6	-13.0	3.00	5.00	14400	24	-2.01	-3.27	9.4	-549	387	2
42	0.70	VE-KR1	691	14	-95.4	-12.4	0.40	5.00	9900	24	-2.02	-2.11	8.7	-475	30	2
43	0.63	VE-KR1	691	17	-100.9	-12.9	0.20	5.00	9900	24	-2.87	-0.67	8.4	-393	30	2
44	1.17	VE-KR1	691	14	-98.8	-12.8	0.20	5.00	9900	24	-2.95	-0.48	8.3	-384	30	2

	A	B	C	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
1	QualityScores	IDCode	Depth(m)	H3(units)	D(prom)	O18(prom)	O2(mg/L)	DrillWater(%)	PumpRate(ml/min)	LagTime(h)	Log pCO2	Log Calcite(SI)	pH(Calc)	Eh(Calc)	PackerDist(m)	Coastal
45	0.48	VE-KR1	883	27	-98.8	-12.8	0.40	5.00	4400	24	-2.81	-0.81	8.4	-411	239	2
46	0.69	VE-KR1	883	19	-97.0	-12.9	0.30	5.00	4400	24	-3.32	-0.23	8.4	-324	239	2
47	0.72	VE-KR4	370	51	-94.4	-13.0	0.01	0.20	37	24	-3.22	-0.21	8.3	-390	40	2
48	1.47	KI-KR1	825	0	-96.0	-12.4	0.38	0.90	15	24	-2.14	-0.76	8.0	-279	12	2
49	0.81	KI-KR1	175	0	-92.7	-12.4	#N/A	1.20	17	24	-2.98	-0.10	8.1	-327	12	2
50	0.83	KI-KR1	822	6	-97.9	-12.8	0.00	10.00	4140	24	-2.88	-0.23	8.2	-379	30	2
51	0.58	KI-KR1	119	8	-95.4	-12.5	0.10	10.00	16430	24	-2.38	-0.44	7.9	-316	158	2
52	0.52	KI-KR1	119	8	-97.9	-12.5	0.20	10.00	16900	24	-2.50	-0.35	7.9	-292	158	2
53	1.02	KI-KR2	220	9	-101.8	-13.5	0.02	0.30	40	24	-3.64	-0.02	8.5	-346	60	2
54	0.48	KI-KR6B	175	34	-95.7	-12.6	0.20	0.60	40	24	-3.35	-0.16	8.5	-320	10	2
55	0.32	SY-KR1	744	7	-92.1	-11.9	0.00	16.00	107	24	-5.17	1.49	7.6	-228	10	2
56	0.39	SY-KR1	744	3	-92.3	-12.2	0.00	11.00	700	24	-5.15	1.32	7.7	-233	10	2
57	1.16	SY-KR1	602	0	-92.9	-12.0	0.00	11.80	120	24	-2.74	0.21	7.6	-322	10	2
58	0.41	SY-KR1	602	4	-93.4	-12.1	0.00	10.80	120	24	-3.46	0.95	7.3	-283	10	2
59	1.04	SY-KR1	602	0	-92.3	-12.1	0.00	12.40	110	24	-3.80	1.05	7.4	-276	10	2
60	0.30	SY-KR1	602	8	-93.6	-12.2	0.00	#N/A	130	24	-3.95	1.09	7.3	-250	10	2
61	1.18	SY-KR1	602	0	-93.0	-12.2	0.00	16.80	120	24	-3.99	0.91	7.4	-243	10	2
62	0.34	SY-KR1	602	6	-90.0	-12.1	0.00	14.00	104	24	-4.25	0.84	7.7	-275	10	2
63	0.42	SY-KR1	178	5	-92.6	-12.1	0.00	10.60	130	24	-3.44	0.81	7.8	-361	10	2
64	0.40	SY-KR1	855	8	-88.8	-12.1	0.90	5.20	1010	24	-2.37	-0.15	7.0	-235	334	2
65	0.55	SY-KR1	610	8	-90.8	-12.1	0.50	3.60	830	24	-1.94	-0.04	7.1	-256	31	2
66	0.51	SY-KR1	610	8	-90.6	-12.1	0.60	10.00	830	24	-2.37	0.21	7.1	-269	31	2
67	0.30	SY-KR1	220	8	-93.3	-12.3	0.00	24.60	2030	24	-1.62	-1.67	8.2	-424	361	2
68	0.64	SY-KR2	455	9	-104.2	-12.8	0.01	2.40	20	24	-3.43	0.85	7.5	-189	80	2
69	1.10	SY-KR6	292	9	-104.7	-12.9	0.03	26.00	30	24	-4.70	1.12	7.9	-178	5	2
70	0.75	SY-KR6	181	34	-94.3	-12.6	0.02	14.00	250	24	-5.04	1.14	8.1	-293	6	2
71	0.93	KLX01	275	8	-89.9	-11.5	0.36	4.60	129	6	-3.72	0.90	7.6	-251	5	1
72	0.65	KLX01	459	8	-94.5	-12.2	#N/A	13.70	138	6	-3.45	0.58	7.6	-229	5	1
73	0.97	KLX01	691	8	-98.8	-11.8	#N/A	1.99	96	6	-3.44	0.03	7.6	-250	22	1
74	0.78	KAS02	208	8	-108.9	-13.9	#N/A	0.81	61	6	-2.77	0.22	7.2	-216	13	1
75	0.50	KAS02	326	8	-99.8	-12.7	#N/A	0.71	5000	6	-3.33	0.21	7.4	-259	36	1
76	0.59	KAS02	466	8	-99.9	-12.8	0.03	0.38	158	6	-4.19	0.81	7.5	-290	5	1
77	1.55	KAS02	533	8	-97.2	-12.3	#N/A	0.28	117	6	-4.25	0.14	7.9	-313	5	1
78	0.95	KAS02	863	8	-96.8	-13.0	0.53	0.22	15200	6	-4.64	0.31	7.8	-254	122	1
79	1.36	KAS02	892	8	-96.8	-13.1	0.36	0.22	135	6	-4.90	0.85	7.7	-247	64	1
80	1.57	KAS03	132	8	-124.8	-15.8	#N/A	0.06	122	6	-3.33	0.18	7.8	-287	5	1
81	0.77	KAS03	209	8	-115.3	-14.6	0.04	#N/A	#N/A	6	-3.11	0.13	7.5	#N/A	26	1
82	0.69	KAS03	250	8	-118.1	-14.5	0.50	1.04	4000	6	-3.25	0.27	7.5	#N/A	3	1
83	0.79	KAS03	360	8	-104.9	-13.3	#N/A	0.83	18000	6	-3.95	-0.06	7.9	#N/A	26	1
84	0.47	KAS03	467	8	-109.6	-13.6	0.30	2.13	16000	6	-3.57	0.23	7.5	#N/A	27	1
85	0.42	KAS03	616	8	-103.4	-13.3	0.39	2.23	18800	6	-4.28	0.23	7.8	#N/A	14	1
86	0.93	KAS03	846	8	-99.7	-13.0	0.45	2.57	13000	6	-4.28	0.31	7.7	-251	312	1
87	1.30	KAS03	931	8	-96.4	-12.7	0.24	0.13	118	6	-3.57	-0.31	7.6	-240	142	1

	A	B	C	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
1	QualityScores	IDCode	Depth(m)	H3(units)	D(prom)	O18(prom)	O2(mg/L)	DrillWater(%)	PumpRate(ml/min)	LagTime(h)	Log pCO2	Log Calcite(SI)	pH(Calc)	Eh(Calc)	PackerDist(m)	Coastal
88	0.90	KAS04	231	4	-84.8	-11.0	0.29	0.16	100	6	-2.53	0.29	7.5	-203	9	1
89	0.75	KAS04	339	8	-99.6	-13.0	0.36	0.52	108	6	-3.25	0.63	7.3	-222	9	1
90	1.17	KAS04	460	8	-92.3	-11.9	0.30	0.08	93	6	-3.98	0.49	7.6	-267	41	1
91	0.53	KAS06	241	4	-94.3	-10.9	#N/A	0.72	15000	6	-2.86	0.49	7.1	-202	73	1
92	1.56	KAS06	341	8	-77.8	-9.2	#N/A	0.03	16300	6	-3.05	0.26	7.2	-223	73	1
93	1.61	KAS06	398	8	-69.2	-7.4	#N/A	0.03	15000	6	-2.94	0.34	7.2	#N/A	17	1
94	1.02	KAS06	521	4	-70.8	-8.2	#N/A	0.05	25000	6	-3.05	0.27	7.2	-231	163	1
95	1.14	KAV01	423	19	-78.0	-10.6	0.18	9	185	6	-2.23	0.06	7.3	-267	5	1
96	1.11	KAV01	527	13	-80.0	-10.9	0.16	10	165	6	-2.25	-0.50	7.4	-293	9	1
97	0.98	KAV01	561	8	-86.0	-11.7	0.10	#N/A	200	6	-2.81	-0.21	7.4	-271	5	1
98	0.90	KAV01	689	3	-92.0	-12.8	#N/A	#N/A	120	6	-2.96	-1.42	7.9	#N/A	109	1
99	0.48	BFI01	289	3	-89.0	-11.8	6.40	#N/A	71	6	-2.33	-0.44	7.2	-127	10	2
100	1.01	BFI01	360	3	-86.9	-11.5	1.76	0.03	185	6	-2.82	0.24	7.1	#N/A	50	2
101	1.32	BFI01	449	3	-88.7	-11.8	8.54	0.02	60	6	-2.65	-0.21	7.3	-117	20	2
102	0.78	KFI01	209	40	-88.0	-11.6	#N/A	#N/A	#N/A	6	-2.19	0.27	7.3	-329	5	2
103	0.46	KFI01	296	40	-87.0	-11.6	#N/A	#N/A	#N/A	6	-2.15	0.21	7.4	-342	5	2
104	0.43	KFI04	250	11	-81.0	-11.5	#N/A	#N/A	#N/A	6	-2.30	0.12	7.7	-362	5	2
105	0.42	KFI04	371	14	-85.0	-10.9	#N/A	#N/A	#N/A	6	-2.29	0.09	7.7	-373	5	2
106	0.87	KFI04	537	10	-85.0	-11.4	#N/A	#N/A	#N/A	6	-2.20	-0.01	7.7	-344	5	2
107	0.50	KFI05	208	7	-86.0	-10.9	#N/A	#N/A	#N/A	6	-2.60	0.14	7.2	-260	5	2
108	0.51	KFI05	300	5	-88.0	-11.8	#N/A	#N/A	#N/A	6	-3.05	0.08	7.3	-278	5	2
109	0.61	KFI07	126	13	-87.0	-11.6	#N/A	#N/A	#N/A	24	-2.36	0.26	7.5	-320	5	2
110	0.83	KFI07	304	3	-90.0	-11.7	#N/A	#N/A	#N/A	6	-3.05	0.96	7.3	-245	5	2
111	0.39	KFI07	325	11	-88.0	-11.8	#N/A	#N/A	#N/A	24	-2.84	0.97	7.2	-276	5	2
112	0.33	KFI07	514	8	-89.0	-11.9	#N/A	#N/A	#N/A	6	-2.77	0.95	7.2	-243	5	2
113	0.71	KFI09	185	3	-84.0	-11.6	#N/A	#N/A	#N/A	6	-2.37	0.23	7.2	-234	5	2
114	0.48	KFI09	363	3	-87.4	-11.1	0.30	#N/A	#N/A	6	-3.35	0.13	7.5	-266	5	2
115	0.54	KFJ02	124	#N/A	-80.5	-11.3	#N/A	1.97	#N/A	6	-2.57	-0.40	8.1	-386	3	2
116	0.38	KFJ04	318	21	-82.6	-11.5	#N/A	4.41	#N/A	24	-2.30	-0.35	7.8	-396	3	2
117	0.61	KFJ04	411	12	-81.6	-11.5	#N/A	3.31	#N/A	6	-3.23	0.40	8.0	-387	3	2
118	0.71	KFJ04	497	6	-84.7	-11.7	0.02	0.71	#N/A	6	-3.17	0.27	8.1	-397	3	2
119	0.53	KFJ07	433	3	-80.1	-11.2	0.04	#N/A	97	6	-3.46	0.24	8.3	-427	3	2
120	0.52	KFJ07	543	3	-81.2	-11.4	0.19	#N/A	87	6	-2.24	-1.05	8.4	-413	3	2
121	0.54	KFJ07	741	#N/A	-80.6	-11.4	0.05	#N/A	103	6	-2.36	-0.68	8.2	-339	39	2
122	0.83	KFJ08	471	8	-79.3	-11.2	0.01	5.52	#N/A	6	-3.50	0.51	8.0	-398	3	2
123	0.76	KFJ08	667	10	-77.8	-10.9	0.02	4.73	#N/A	6	-3.89	0.87	8.1	-404	3	2
124	0.66	KGI02	179	3	-90.4	-12.6	#N/A	0.16	211	6	-3.36	0.15	8.3	-388	3	2
125	0.65	KGI02	329	3	-90.1	-12.6	0.05	0.24	222	6	-3.66	0.42	8.4	-422	3	2
126	0.58	KGI02	401	3	-91.4	-12.7	0.06	0.39	178	6	-3.48	0.26	8.4	-409	3	2
127	0.60	KGI02	545	3	-89.5	-12.4	#N/A	0.39	206	6	-3.69	0.43	8.4	-431	3	2
128	0.86	KGI02	603	3	-92.7	-12.7	0.01	0.24	190	6	-3.53	0.34	8.3	-413	3	2
129	0.59	KGI04	223	5	-89.7	-12.6	0.05	1.50	145	6	-3.94	0.49	8.5	-406	3	2
130	0.54	KGI04	405	8	-99.4	-13.6	0.75	11.03	98	6	-5.20	0.28	9.1	-475	3	2

	A	B	C	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
I	QualityScores	IDCode	Depth(m)	H3(units)	D(prom)	O18(prom)	O2(mg/L)	DrillWater(%)	PumpRate(ml/min)	LagTime(h)	Log pCO2	Log Calcite(SI)	pH(Calc)	Eh(Calc)	PackerDist(m)	Coastal
131	0.77	KGI04	513	49	-94.1	-12.9	0.02	0.32	143	6	-3.20	0.23	8.0	-417	3	2
132	2.13	KGI04	617	10	-100.8	-13.8	3.00	29.94	1	6	-3.23	-0.33	8.2	#N/A	3	2
133	0.50	KKA03	233	77	-59.0	-8.8	#N/A	#N/A	#N/A	6	-1.29	-1.17	7.5	-362	3	2
134	0.50	KKA04	227	58	-69.0	-10.0	#N/A	#N/A	#N/A	6	-1.96	-0.07	7.4	-285	3	2
135	0.58	KKA04	398	60	-71.0	-9.9	#N/A	#N/A	#N/A	6	-1.96	-0.04	7.3	-262	3	2
136	0.58	KKR01	104	3	-78.0	-10.3	#N/A	#N/A	#N/A	6	-2.06	-0.37	7.7	#N/A	3	1
137	0.45	KKR01	265	3	-77.0	-10.4	#N/A	#N/A	#N/A	6	-2.62	0.11	7.8	#N/A	3	1
138	0.42	KKR01	407	3	-79.0	-10.7	#N/A	#N/A	#N/A	6	-2.86	0.22	7.9	#N/A	3	1
139	0.49	KKR01	492	3	-83.0	-10.4	#N/A	#N/A	#N/A	6	-2.54	-0.13	7.9	#N/A	3	1
140	0.63	KSV04	97	5	-90.0	-12.5	#N/A	1.02	198	6	-3.13	0.19	8.0	-294	3	2
141	0.60	KSV04	377	3	-95.3	-13.2	0.02	1.89	198	6	-2.18	-1.21	8.4	-395	3	2
142	0.53	KSV04	431	3	-95.0	-13.0	0.11	1.02	208	6	-4.02	0.80	8.2	-379	3	2
143	0.63	KSV04	631	3	-95.4	-13.1	#N/A	0.63	170	6	-3.67	0.48	8.2	-377	3	2
144	0.61	KSV05	161	33	-92.2	-12.8	0.15	1.58	70	6	-1.50	-2.93	8.8	-519	3	2
145	0.47	KTA01	497	153	-98.0	-13.8	#N/A	#N/A	250	6	-3.96	-0.82	9.2	-463	3	2
146	0.43	KTA01	677	115	-97.1	-13.6	0.62	#N/A	148	6	-5.08	0.23	9.2	-546	46	2

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B L Josefson¹, L Karlsson², H-Å Häggblad²

¹ Division of Solid Mechanics, Chalmers University of Technology, Göteborg, Sweden

² Division of Computer Aided Design, Luleå University of Technology, Luleå, Sweden

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Hydrothermal field test with French candidate clay embedding steel heater in the Stripa mine

R Pusch¹, O Karnland¹, A Lajudie², J Lechelle², A Bouchet³

¹ Clay Technology AB, Sweden

² CEA, France

³ Etude Recherche Matériaux (ERM), France
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R Pusch¹, O Karnland¹, A Lajudie², A Decarreau³,

¹ Clay Technology AB, Sweden

² CEA, France

³ Univ. de Poitiers, France

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Fredrik Brandberg¹, Bertil Grundfelt¹, Lars Olof

Höglund¹, Fred Karlsson²,

Kristina Skagius¹, John Smellie³

¹ KEMAKTA Konsult AB

² SKB

³ Conterra AB

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Thomas Eliasson

Chalmers University of Technology and University of Göteborg, Department of Geology, Göteborg, Sweden

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L Romero, L Moreno, I Neretnieks

Department of Chemical Engineering,

Royal Institute of Technology, Stockholm, Sweden

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Joel Geier

Golder Geosystem AB, Uppsala

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² SKB

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Department of Geology, Chalmers University of Technology and University of Göteborg

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Trygve E Eriksen¹, Pierre Ndalamba¹, Daqing Cui¹,
Jordi Bruno², Marco Caceci², Kastriot Spahiu²
¹ Dept. of Nuclear Chemistry, Royal Institute of
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² MBT Tecnologia Ambiental, Cerdanyola, Spain
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