

# DESIGN CONSIDERATIONS FOR THE ACQUISITION OF HYDROCHEMICAL DATA FROM DEEP BOREHOLES

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## Abstract

Deep (>300 m) subsurface hydrochemical data are important components of geological investigations of potential radioactive waste disposal sites. These data can be interpreted to yield information that supports conceptual hydrogeological models, constrains palaeohydrogeological evolution and characterises subsurface hydrochemical conditions of a site. The most important sources of these data are the analyses of groundwater samples collected during extraction tests performed in boreholes either during drilling or after drilling has been completed. To maximise the information obtained from their interpretation, the quality and quantity of hydrochemical data obtained should be such that they are representative of the compositions of the in-situ groundwaters, the in-situ location of all groundwaters should be known, and the key trends in groundwater compositions should be identifiable from the data set.

The design of deep borehole-based hydrochemical data acquisition programmes to meet such objectives is a complex task. It is useful to simplify the design process by focusing attention on those activities and parameters that are most likely to affect the quality and quantity of hydrochemical data obtained from the final implemented design. In this paper we examine those design parameters associated with drilling (cutting method, drilling fluids, flushing method, drill string and bottomhole assembly), fluid extraction testing (timing, test tools, fluid extraction method), sampling (sampling locations, timing of sampling, numbers of samples, sample collection methods), and sample analysis (analytical precision and accuracy, location and timing of analyses) activities. For each parameter we discuss the design options available, and identify those with features that are most likely to be beneficial or detrimental to the quality and quantity of hydrochemical data.

Preferred design options have been identified where possible. However, each investigation will have a number of external constraints associated with it arising from either the investigation itself, the site or available technology. As a result, depending on the circumstances of each investigation, it may not be possible to include all the preferred design options into a final design.

## 1. Introduction

An important objective of geological investigations of potential radioactive waste disposal sites is the collection of hydrochemical (groundwater composition) data from deep (>300 m) locations at the site. The interpretation of these data can be used to yield information that supports conceptual hydrogeological models (eg Nirex, 1998a), constrains palaeohydrogeological evolution (eg Fontes, 1994) and characterises subsurface hydrochemical conditions of a site (eg Pearson and Scholtis, 1993).

The principal sources of these data, and the subject of this paper, are analyses of groundwater samples collected during extraction tests performed in boreholes either during drilling or after drilling has been completed. To maximise the information obtained from interpretation, the quality and quantity of the hydrochemical data should be such that they are representative of the compositions of the in-situ groundwaters, the in-situ location of all groundwaters should be known, and the key trends in groundwater compositions should be identifiable from the data set. The quality and quantity of hydrochemical data obtained are largely determined by the activities associated with the drilling of the borehole, extraction of groundwater from the formation, and collection and analysis of groundwater samples (primary activities).

The design of primary activities to obtain hydrochemical data will normally be constrained by a number of factors. These may be associated with the investigation itself (eg financial, programme, priorities placed on the acquisition of different data, limitations on borehole locations, etc), the site (eg local geological conditions, groundwater compositions, etc), or they may be of a technical nature (eg availability of equipment, techniques, methods, etc). Under such circumstances, the designer needs to consider which design parameters will most influence the quality and quantity of hydrochemical data obtained and what options are available for each parameter. The designer can then choose options that will best provide the data required given the constraints.

Based on our experiences on the UK Nirex investigation at Sellafield, and building on the experiences of other earlier investigations (eg Bottomley et al., 1984; Smellie et al., 1985; Haug, 1985; Smellie and Wikberg, 1991; Ross and Gascoyne, 1995), in this paper we will identify the key design parameters for the primary activities and discuss design options available for each parameter. For each option, we will also identify those with features that are most likely to be beneficial or detrimental to the quality and quantity of hydrochemical data obtained, and where possible, we will identify those design options that are preferred for deep borehole-based hydrochemical data acquisition programmes.

## **2. Drilling Design**

### **2.1. Cutting Method**

Given the typical depths of investigation boreholes, two cutting techniques may be considered: rotary or percussive drilling, and coring. Both methods may provide similar penetration rates but coring is preferable because the finer cuttings produced allows lighter drilling fluids to be used. As discussed below, this minimises borehole pressures, and hence contamination of the groundwater with drilling fluid. Collection of core is beneficial to water-rock interaction studies, may allow core pore fluid data to be obtained and helps provide information about the condition of the rock in the proposed fluid extraction test interval (eg the location of potential flowing features and suitable packer seats).

### **2.2. Drill fluids and flushing method**

Drilling fluid losses to the host rock are most likely to occur at any points where the pressure in the borehole exceeds that in the formation. The highest borehole pressures occur at the drill bit where some losses are inevitable. Losses may be reduced using drilling fluid additives or by keeping borehole pressures as low as possible. The latter can be accomplished by the use of low density fluids or artificial lifting (eg gas injection).

Constituents in groundwaters affected by drilling fluids can be categorised as being affected by either mixing-type contamination or reaction-type contamination (McCartney and Solbé, in prep.). Reaction-type contamination may result from a variety of interactions involving the drilling fluid, groundwater, drilling fluid/groundwater mixtures, formation minerals, secondary reaction products and drilling fluid debris (see Figure 2-1). A number of studies have identified the potential for drilling fluid materials to be retained in the formation after they have been lost (eg Graham and Johnson, 1991). Baeyens and Bradbury (1991) have shown how even 'pure' groundwaters can have their compositions modified during transport to the borehole through reactions with drilling fluid-affected fracture surfaces. The use of complex drilling fluids to control drilling fluid losses (eg bentonites, polymers, etc) should be avoided where possible because although mixing-type contamination effects can be corrected (see below), drilling fluid-groundwater-formation mineral reactions are poorly understood. Thus, it is difficult to attempt to make corrections to reaction-type contaminated groundwater composition data. The use of complex drilling fluids may also lead to plugging of fractures.

Low density drilling fluids may include either air or low salinity water. In deeper (>250m) or inclined holes the cuttings lifting characteristics of air can be poor (eg Smellie and Wikberg, 1991) which can jeopardise the drilling of the hole itself. Use of air as the drilling fluid can also lead to oxidation of the formation and groundwaters, particularly at greater depths where air injection pressures are high (Bottomley et al., 1984; Smellie and Wikberg, 1991). A compromise drilling fluid would be low salinity water which has better lifting characteristics than air and its interactions with groundwaters and formation minerals are better understood than drilling fluids with additives. It is preferable to choose a low salinity water with a composition that will

least affect the groundwater composition by mixing or reaction.

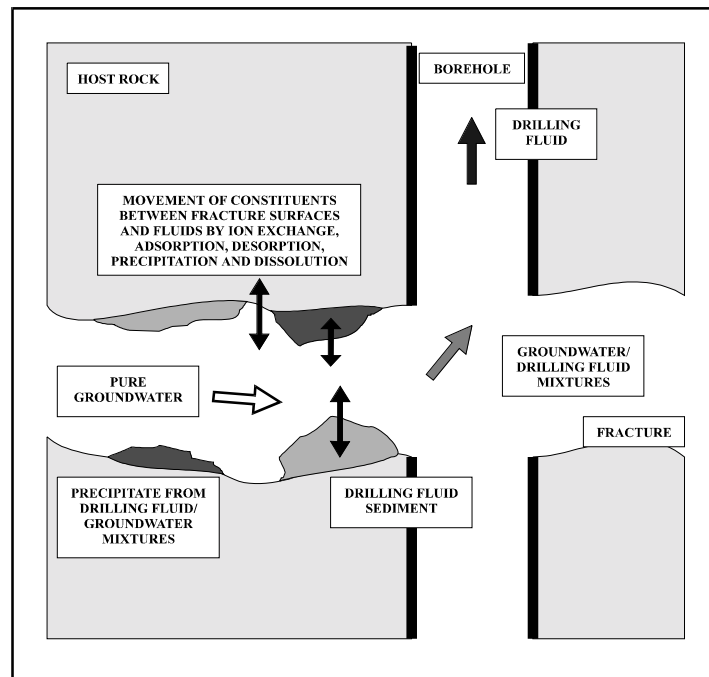


Figure 2-1 Schematic representation of interactions occurring between drilling fluids and groundwaters following losses of drilling fluid to the formation and during their subsequent extraction.

Two methods have been used to artificially reduce borehole pressures during drilling: normal (eg Almén and Zellman, 1991) and reverse (eg Ljunggren, 1993) air-assisted drilling fluid circulation. Although drilling fluid contamination of groundwaters is minimised with the normal method, this effect is not avoided (Nirex, 1998b). There are practical limitations on the use of the reverse method (eg fluid flow from the formation needs to be fairly continuous and uniform; Ljunggren, op. cit.). With both methods there is an increased risk of disturbing the initial distribution of groundwaters due to the net inflow of groundwater to the borehole during drilling. There is also a risk of cross-flow contamination of sections of the formation during breaks in drilling. However, both risks can be minimised by using drill-and-test methods (see below), continuous drawdown below minimum formation pressure and surface read-out downhole pressure monitoring. With both methods, by monitoring the composition of drilling fluid produced from the borehole, the location of significant inflows of groundwater to the borehole may be identified and can aid the selection of fluid extraction test zones.

As drilling fluid contamination of groundwaters is to be expected, the drilling fluid should include an inert tracer. The presence of inert tracer in a sample can demonstrate the presence of mixing-type drilling fluid contamination which itself identifies the potential for reaction-type contamination. Control of the inert tracer and drilling fluid composition and collection and analysis of drilling fluid samples during drilling will allow the groundwater compositions of those constituents only affected by mixing with drilling fluids to be estimated (eg  $^3\text{H}$ , Cl, Br, etc; McCartney and Solbé, in prep.). Such data will also assist with the deconvolution of drilling fluid/groundwater reaction effects. Graham and Johnson (1991) have suggested the use of 'reactive' tracers in

drilling fluids to trace reaction-type contamination although such a technique would be limited to those constituents that undergo similar reactions to the tracers used. Where groundwater flows into the borehole during drilling, as with air-assisted methods, control of the drilling fluid and tracer composition can be difficult. If water supply and disposal are not limited, these problems can be avoided through the use of open-loop drilling fluid circulation (ie drilling fluid is not re-circulated into the borehole).

### **2.3. Drillstring and Bottom Hole Assembly**

Core may be recovered during drilling either conventionally where the core barrel is removed with the drillstring or by wireline recovery, where the core can be recovered without removing the drillstring. Wireline recovery minimises movement of the drill string in and out of the borehole and therefore reduces the potential for drilling fluid invasion of the formation and for cross-flow contamination due to surging and suction effects.

Debris from the materials from which the drillstring, downhole tools and bits are made (including lubricants) may be deposited on the borehole walls, settle to the bottom of the borehole or may be carried into the formation with drilling fluids. Groundwaters entering the borehole during extraction testing may react with this debris. As a general principle, any drilling related materials should be tested for their potential reactivity with the anticipated groundwaters before drilling proceeds. Drilling equipment should be selected so as to minimise the potential impact on chemical constituents of interest. The same can be said of all equipment used during testing, sampling and analysis. Consideration should be given to the use of less reactive materials such as stainless steel, PVC or teflon coated equipment, solid lubricating materials such as PTFE, etc.

### **2.4. Hole size**

Small diameter holes are preferable because the annulus between the borehole wall and drill string is likely to be small. This allows high fluid return velocities to be achieved, which assists the removal of cuttings and improves the performance of lower density drilling fluids. There is also a smaller volume of drilling fluid in circulation which simplifies water supply and disposal in open-loop circulation systems. A small hole size will also reduce the volume of borehole associated with a section to be tested (see below).

## **3. Extraction tests**

### **3.1. Timing**

There are two general approaches to the timing of testing in relation to drilling activities. Testing may either take place at progressively greater depths as the borehole is drilled (drill-and-test method) or a relatively large section of the borehole will be drilled and subsequently tested (drill-then-test method). The former approach is preferable with respect to the quality of groundwater samples because the longer a section of borehole remains untested, the greater the potential for drilling fluid contamination of

groundwaters and the associated disturbance of the groundwater distribution adjacent to the borehole. With either approach, extended breaks during or after drilling may increase the risk of cross-flow contamination via the open hole. The latter can be avoided through monitoring the formation pressure with depth, maintaining a drawdown on the borehole greater than the lowest formation pressure, and/or through the separation of active zones by packers.

The section of borehole to be tested should contain fractures or porous formations capable of having fluids extracted from them with the equipment and extraction methods available if groundwater samples are to be collected. Production logs (electrical conductivity, temperature, flow) used in conjunction with geophysical logs on borehole sections are the preferred method of identifying such features. For the drill-test approach, frequent production logging may be impractical. In such cases, changes in drilling parameters (eg drilling fluid losses and gains) or identification of potential flowing features in core can be useful but are less reliable.

### **3.2. Test tools**

Testing a small section of the borehole will minimise the possibility of sampling more than one compositional type of groundwater (ie artificially mixing the groundwaters and disturbing the original groundwater distribution). This can be achieved using straddle-packers positioned around the zone to be tested or, if the test zone is at the bottom of the borehole, a single packer located just above the zone to be tested. The packers may be set via a surface inflation line or by rotation. Inflation by pressurisation of the test string with water can result in contamination of groundwater samples during short duration, lower flow rate extraction tests when downhole samplers need to be used (see below). The inclusion of a shut-in valve in the test tools provides further sampling opportunities (see below) and allows the formation pressure to be measured. The risk of groundwater contamination through packer leakage can be minimised through the use of guard packers and selection of packer seating zones using information from core or televiewer logs. Packer leakage can be detected by monitoring the pressure in the guard zones and test sections. Surface readout of pressure allows a more rapid response to detected problems. The reduction of dead volumes between the packers will minimise diffusive contamination of groundwater samples. Dispersive contamination will also be minimised where several minor fractures intersect the borehole in addition to the major fracture. By limiting the test string diameter, groundwater samples will be more quickly produced at the surface, minimising groundwater contact with the test string.

### **3.3. Fluid extraction method**

If the formation is not artesian, the fluid can be extracted from the formation and borehole using gas-lift (eg air, nitrogen), mechanical bailing devices (eg swabbing, bailers) or submersible pumps. Greater rates of extraction tend to be achieved using gas-lifts and high capacity pumps. However, if samples are to be collected at the surface during extraction tests (see below), each of the methods may affect the groundwater composition. For example, gas-lifting strips the groundwaters of dissolved gases, contaminates them with the gas used for lifting and can warm or cool the groundwaters depending on the gas and groundwater temperatures. Air contamination, pressure loss and temperature change are common problems with groundwaters extracted by

swabbing and bailing. With this method, 'drain back' of fluid into the test string can result in air contamination of samples subsequently collected downhole (Ross and Gascoyne, 1995). Gas loss through de-pressurisation and temperature changes are common in artesian or pumped groundwater samples.

Each extraction method results in a decrease in test section pressure relative to that in the formation (ie a pressure drawdown). Increased drawdown on the test section increases the risk of packer leakage (sample contamination) and borehole breakout (potential loss of borehole). Similarly, it increases the risk of disturbing the natural distribution of groundwaters in the formation. In extreme cases, reduction of formation pressure may lead to outgassing and changes in groundwater composition in the formation. It is therefore preferable to limit drawdowns so that they do not exceed the in-situ gas pressure in the groundwaters.

## **4. Sampling**

### **4.1. Sampling locations**

Groundwater samples can be collected from four generic locations during extraction tests; downhole in wireline samplers in the test string just above the test section, downhole in samplers within the test section tools, at the surface next to the wellhead, and from the test string at the surface as it is removed from the borehole at the end of the test. Downhole wireline samplers provide the best quality samples if they are obtained below any disturbances caused by the extraction method. They have limited contact time with downhole equipment and may also be the only method of collection under low flow rate extraction conditions. Samplers are available that can maintain the samples under pressure up to the point of sample analysis. However, sample size is limited (typically less than 5 litres) making multiple sampling runs necessary. The act of running the samplers into the test string can lead to artificial mixing of the fluids in the test string which can be problematic in low flow rate extraction tests. Large samples can be obtained from the surface or test string without contacting the atmosphere if de-gassing, de-pressurisation or extended contact with the test string is not problematic for the constituent of interest. All samples are affected by temperature changes during transport out of the formation although, if the temperature changes are measured, any changes in groundwater composition (eg pH) can be calculated and corrected for (eg Pearson et al., 1989).

### **4.2. Timing of sampling, numbers of samples and sample collection methods**

A groundwater 'sample' is often made up of a set of samples collected at approximately the same time but from different locations. Analyses for each constituent are performed on those samples for which the best quality data can be obtained. There are two general approaches that are adopted with respect to the timing of collection of sample sets. A series of sample sets may be collected over time during the test (time series sets) or one or more sample sets can be collected at the end of the test (end of test sets). Time series sets can be used for extrapolating the groundwater composition where a drilling fluid tracer is used. This can keep test durations short and minimises disturbance to the

groundwater distribution but extrapolation techniques have their limitations (see above). The end of test approach seeks to obtain what can be considered to be pure groundwater samples (ie when, for the constituents of interest, drilling fluid contamination is negligible). Test durations tend to be longer and the risk of disturbance to the groundwater distribution is increased. In addition, even when drilling fluid tracer levels are low, drilling fluid contamination of samples may still occur (eg Baeyens and Bradbury, 1991). Alternative methods of assessing drilling fluid contamination clean-up (eg achievement of a steady extracted fluid composition or extraction of pre-calculated volumes) can be misleading (Graham and Johnson, 1991).

Alteration or contamination of samples during collection and prior to analysis can be minimised through judicious selection of sample collection methods. This includes immediate post-collection treatment of samples (eg transfer of samples between vessels, addition of preservatives, pre-concentration, filtration, storage, etc).

## **5. Sample Analysis**

### **5.1. Analytical precision and accuracy**

Although short term precision can be measured for quality control purposes, the most meaningful measure of analytical precision is long term precision determined by analysis of an 'internal standard' with each batch of analyses (Taylor, 1987). As well as being a quality control tool it allows confident comparison of data obtained throughout a site investigation. Internal standards should preferably have compositions similar to the samples being analysed.

Accuracy of the chosen analytical methods may be assessed through their use to measure (a) international reference standards, (b) samples used in inter-laboratory analysis comparison schemes, (c) laboratory prepared reference standards, or (d) spiked samples (Taylor, 1987). Again, preferably these should have compositions similar to the samples collected from the site. This is rarely the case for the former two options. For the latter two options, demonstration of accuracy will normally be retrospective. In any event, assessment of the accuracy of measurements will require expert judgement.

### **5.2. Location and timing of analyses**

Ideally, samples should be analysed in a location that (a) minimises alteration or contamination of the sample after collection, (b) is suitable to the timing of use of the analytical results and (c) is appropriate to the analytical method. The four general analytical locations are: downhole in the test string or test tools, at the wellhead, in an on-site laboratory or in an off-site laboratory. Examples of constituents that may be measured downhole are Eh and pH (eg Almén et al., 1986), each of which may change during transport to the surface during extraction tests due to interaction with test string and the atmosphere, and temperature and pressure changes. These constituents and others (eg electrical conductivity, dissolved oxygen, etc) are also often measured at the wellhead (eg Almén et al., 1986). Due to equipment and calibration problems, there is some debate about whether downhole Eh and pH measurements are better than the

wellhead measurements (Whitaker et al., 1994). Where sample contamination or alteration (eg microbial activity, atmospheric effects) may affect particular constituents (eg alkalinity,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{NO}_3$ , etc) soon after collection or where the data is needed for decision-making purposes (eg drilling fluid tracer), analyses are best performed on-site soon after sample collection. Where it is possible to maintain samples in a stable condition for particular constituents for a relatively long period, analysis for these constituents may be performed on-site or off-site some time after collection.

## 6. Conclusions

The design of activities to acquire hydrochemical data from boreholes is a complicated task. However, this task can be simplified if (a) those design parameters that are most likely to affect the quality and quantity of hydrochemical data obtained can be identified, (b) the design options under each parameter can be identified, and (c) the potential impact of these different options on the data can be assessed. This information can allow the designer to focus on design solutions that best match the external constraints associated with the investigation itself, the site and available technology.

## References

- Almén, K-E., Andersson, O., Fridh, B., Johansson, E., Sehlstedt, M., Gustafsson, E., Hansson, K., Olsson, O., Nilsson, G., Axelsen, K., 1986. Site investigation equipment for geological, geophysical, hydrogeological and hydrochemical characterisation. Swedish Nuclear Fuel and Waste Management Co., SKB, Technical Report TR 91-22, Stockholm, Sweden.
- Almén, K-E, Zellman, O., 1991. Aspö hard rock laboratory. Field investigation methodology and instruments used in the pre-investigation phase. Swedish Nuclear Fuel and Waste Management Co., SKB, Technical Report TR 91-21, Stockholm, Sweden.
- Baeyens, B., Bradbury, M. H., 1991. Characterisation of downhole water samples taken during pumping tests from borehole SB4, Wellenberg: Can the groundwater chemistry be deduced from such measurements? Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) Internal Report 91-38, Wettingen, Switzerland.
- Bottomley, D. J., Ross, J. D., Graham, B. W., 1984. A borehole methodology for hydrogeochemical investigations in fractured rock. *Water Resources Res.*, 20, p 1277-1300.
- Fontes, J-Ch., 1994. Isotope palaeohydrology and the prediction of long-term repository behaviour. *Terra Nova*, 6, p 20-36.
- Graham, D. L., Johnson, V. G., 1991. Effects of fluid rotary drilling on hydrochemical sampling results from deep boreholes in fractured Columbia River Basalt. *J. Hydrol.*,

128, p 171-212.

Haug, A., 1985. Feldmethoden zur grundwasser-entnahme aus tiefbohrungen und zur hydrochemischen überwachung der bohrspülung. Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) Technical Report 85-07, Switzerland.

Ljunggren, C., 1993. Core drilling by reverse flushing - a new drilling concept for small diameter holes. Swedish Nuclear Fuel and Waste Management Co., SKB, Technical Report TR 93-30, Stockholm, Sweden.

McCartney, R. A., Solbe, M. J. de L-G, in preparation. Use of tracers in drilling muds to allow the estimation of in-situ formation water compositions from drilling-mud-contaminated formation water samples.

Nirex, 1998a. Sellafield geological and hydrogeological investigations. The hydrochemistry of Sellafield: 1997 update. UK Nirex Limited Science Rept. SA/97/089.

Nirex, 1998b. Sellafield geological investigations: Acquisition of deep borehole groundwater compositions. UK Nirex Limited Science Report SA/97/072.

Pearson, F. J., Lolcama, J. L., Scholtis, A., 1989. Chemistry of waters in the Böttstein, Weiach, Riniken, Schafisheim, Kaisten and Leuggern Boreholes: A hydrochemically consistent data set. Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) Technical Report 86-19, Wettingen, Switzerland.

Pearson, F. J., Scholtis, A., 1993. Chemistry of reference waters of the crystalline basement of northern Switzerland for safety assessment studies. Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) Technical Report 93-07, Wettingen, Switzerland.

Ross, J. D., Gascoyne, M., 1995. Methods for sampling and analysis of groundwaters in the Canadian Nuclear Fuel Waste Management Program. Atomic Energy of Canada Limited Technical Record TR-588, COG-93-36.

Smellie, J. A. T., Wikberg, P., 1991. Hydrochemical investigations at Finnsjön, Sweden. *J. Hydrol.*, 126, p 129-158.

Smellie, J. A. T., Larsson, N-A., Wikberg, P., Carlsson, L., 1985. Hydrochemical investigations in crystalline bedrock in relation to existing hydraulic conditions: Experience from the SKB test-sites in Sweden. Swedish Nuclear Fuel and Waste Management Co., SKB, Technical Report TR 85-11, Stockholm, Sweden.

Taylor, J. K., 1987. Quality assurance of chemical measurements. Lewis Publishers Inc., 328 pp.

Whitaker, S. H., Brown, A., Davison, C. C., Gascoyne, M., Lodha, G. S., Stevenson, D. R., Thorne, G. A., and Tomsons, D., 1994. AECL strategy for surface-based investigations of potential disposal sites and the development of a geosphere model for a site. Swedish Nuclear Fuel and Waste Management Co., SKB, Technical Report TR 94-18, Stockholm, Sweden.