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地下水の地球化学データに関する品質分類手法の構築

（核燃料サイクル開発機構 契約業務報告書）

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要旨

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本報告書は，地下水の地球化学データを品質評価するために，品質分類モデルを作成して，このモデルを用いた品質評価手法の開発を行なった結果について取りまとめたものである。

東濃地科学センターでは，これまで（平成15年度）に地下水の地球化学データの品質を評価するために，予察的な品質評価方法について検討してきた。この方法は，個々の評価指標に対してデータを点数化（スコア化）させて，その合計点によってデータの品質をランク付けする方法である。しかし，この方法には，高得点の指標によって，低得点の指標が判りにくくなってしまうこと，評価指標に関する情報が欠如・不足しているデータの品質が評価できないこと等の制限や問題が含まれている。

地下水の地球化学データの品質を分類する新たなシステムの構築に，ESL（Evidence Support Logic）を用いることにより，上記の制限を除去することができる。この手法は，ある仮説が正しいあるいは信頼できるということを，各評価項目における証拠によって支持または否定される程度を見積もるものであり，様々な定性的・定量的な証拠が総合的に評価される手法である。本手法では対象としている仮説と，観察結果や定量的データに対応した証拠との関連性を表現するプロセスモデル（通常は，幾つかの中間階層のプロセスを経た関係を示すモデル）が構築される。モデルを通して，証拠による支持または否定の程度が上位階層に伝播する計算を行う。したがって本手法は、個々の評価指標に対する品質スコアの単純な足し合わせに基づくものではない。

本手法では，地下水の地球化学データが原位置の状態を表しているという仮説を支持する証拠と否定する証拠を，それぞれ独自に評価している。支持または否定のいずれの証拠も，0～1の間の数値によって表される。データの品質の情報が欠如している場合には，この状態が，「1－支持の証拠－否定の証拠」として数値で表される。このように本モデルでは，品質に関しての情報が十分に存在していてデータの品質が低いことが示されている状況と，品質情報が欠如している状況とは区別される。

作成した品質分類モデルを，広域地下水流動研究および超深地層研究所計画の調査で得られた既往の地下水データ（Furue et al., 2004, 古江他, 2005, 彌榮他, 2004）に適用させて，地下水の地球化学データを品質評価した。評価は，溶解度評価に関する既往

の感度解析結果（Metcalfe et al., 2004）によって，評価すべき重要な地球化学パラメータとされる，以下のパラメータについて実施した。

・Eh

・pH

・酸化還元に関わる鉄成分（Fe^{2+}, Fe^{3+}）

・還元に関わる硫黄成分（HS^-）

・アルカリ度

・炭酸成分(TIC, HCO_3^-, CO_3^{2-}, TOC)

・主要陽イオン(Na^+, K^+, Ca^{2+}, Mg^{2+})

・主要陰イオン(Cl, SO_4^{2-}, PO_4)

pH の測定値，Eh の測定値，酸化還元状態に鋭敏な微量元素の分析値，および無機炭素化学種の分析値について，各々の品質を評価するための個別のプロセスモデルを作成した。pH の測定値の品質を評価するモデルは，主要な陽イオン・陰イオンおよび酸化還元状態にあまり鋭敏でない微量元素の品質評価にも適用できる。

品質評価の結果，ボーリング時の掘削水の残留に関わる条件・環境が，地下水試料の品質に対しては，大きな影響を与え得ることが判明した。したがって調査に際しては，特に上記の条件・環境に関わる情報を，精度良く適切に取得する必要がある。

本業務で作成した品質分類モデルでは，新たな品質情報を評価項目として追加することが可能であるため，取得するデータ・情報の条件に応じた品質分類モデルの改良が可能である。また，それぞれの調査段階や調査条件に応じた取得すべきデータの品質について，国内外の専門家のコンセンサスを得るために，本モデルでは彼らの意見を反映させて適宜改訂することも可能である。

本報告書は，三菱商事株式会社が核燃料サイクル開発機構との契約により実施した業務成果を取りまとめたものである。

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Summary

This report describes the development of a method for the classification of geochemical data quality. The project had four tasks: (1) review of quality information; (2) development of Evidence Support Logic (ESL) models; (3) development of rules for choosing parameter values; (4) classification of existing data.

During H15, JNC developed a preliminary system for classifying groundwater chemical data according to its quality. This system gives a very general indication of data quality, but has a number of limitations. Notably, it is based on adding together scores for individual quality indicators, so that high scores given by some indicators tend to compensate for low scores given by other indicators. Additionally, the system does not distinguish between cases where data quality is poor and cases where data quality is unknown. A further limitation is that the system is based on only a small number of the quality indicators that could be used.

By using ESL to develop a new system for classifying geochemical data quality, these limitations can be avoided. This methodology involves weighing evidence for and against a particular hypothesis being true or reliable. Varied evidence, which may be quantitative or qualitative, can be evaluated in an integrated fashion. A process model is constructed to link a hypothesis of interest to evidence corresponding to observations and quantitative data, usually via intermediate processes. An arithmetical approach is then used to propagate evidence through the model. Thus, the approach does not rely on simple addition of quality scores for individual parameters.

In this project, evidence for and evidence against the hypothesis that groundwater chemical data represent in-situ conditions are evaluated independently. Both kinds of evidence are represented using numerical scales from 0 to 1. Lack of information about data quality is then represented by 1 – evidence for – evidence against. In this way the situation where the available information indicates low data quality is distinguished from the situation in which there is no quality information.

Separate process models have been constructed to evaluate the quality of each of pH measurements, Eh measurements, redox-sensitive trace element analyses and analyses of species of inorganic carbon. The model for evaluating the quality of pH data could also be applied to evaluate the quality of major cations and anions and non-redox sensitive trace elements.

These process models have been applied to data from boreholes.The process models provide a visualisation of data quality judgements that may be appraised rapidly. The models can be revised readily as and when additional quality information becomes

available, or to reflect the differing opinions of different experts concerning data quality.

It is suggested that the process models should be reviewed and revised as necessary by different experts, so as to build a consensus about what levels of data quality are desirable and attainable.

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1 Introduction

1.1 Purpose of the report

Quintessa Japan has developed a quality classification system for the hydrogeochemical data obtained in the Tono are by JNC. The project involved the following tasks:

- ▲ Task 1. Review of quality information
- ▲ Task 2. Development of Evidence Support Logic (ESL) models
- ▲ Task 3. Development of rules for choosing parameter values
- ▲ Task 4. Classification of existing data

1.2 Need for a quality classification system

The first step when interpreting any groundwater chemical data is to evaluate the quality of the data. Ideally, it should be established to what extent the chemical data reflect in-situ (that is natural, undisturbed) conditions.

Many research programmes investigating deep groundwater systems have developed systems to evaluate the quality of the geochemical data obtained (e.g. Laaksoharju et al., 1993; Nirex, 1996, 1997; Pearson et al. 2003). A preliminary groundwater quality classification scheme has also been developed by JNC for the groundwater data obtained in the Tono area. This latter scheme was based partly upon the approach adopted in Sweden and Finland (c.f. Laaksoharju et al., 1993). However, the investigations in the Tono area have been more varied in character than in most other investigations. Initially uranium exploration activities produced groundwater data. Subsequently groundwaters were also sampled and analysed during the Tono Natural Analogue Project (TAP), during regional hydrogeological investigations. Groundwater has also been sampled at two separate sites (Shobasama and Togari) during investigations for the Mizunami Underground Laboratory (MIU) . These investigations in the Tono area have proceeded for almost 30 years and the quality information recorded with the groundwater data has varied in quantity and quality. The most recent investigations have been very well documented, but very little information is available concerning the borehole drilling, sampling and analytical methods employed during the earliest investigations related to uranium exploration.

Therefore, there remains a need to develop a system for classifying and recording the quality of geochemical data that can be applied to all these diverse sets of hydrogeochemical data. The system should ensure that:

- quality information is recorded consistently (that is, different samples sampled under similar conditions will be assigned the same quality designation);
- quality information is recorded objectively (that is, different people applying the same quality classification system to the same samples will produce the same result);
- the quality information can be used for different purposes (i.e. recognising that the 'quality' of data depends on how the data are to be used);
- recognizes the difference between samples for which the quality is unknown and samples for which the quality is clearly poor (i.e. does not cause data to be always assumed to be poor, simply because insufficient quality information are available).

1.3 Characteristics of a quality scoring system

1.3.1 General characteristics of scoring systems

Quality scoring systems that have been developed during other programmes are essentially procedures that can be used to rank the samples or individual data in a set. Such a system has the following general characteristics:

- It is a measure of reliability or 'representativeness' for in-situ groundwater composition of a water sample or data point for an individual determinand.
- The measure can be qualitative or semi-quantitative, but with groundwater data, especially hydrochemical data, ***it can rarely be regarded as being quantitative***.
- A quality scoring system should be defensible as being as objective as possible.
- Quality scores are usually pragmatic estimates, for which the scales are relative within a particular data set.

The main requirements from such a data scoring system are that it should:

- identify the most reliable samples and analyses overall, for general interpretation of hydrochemical and isotopic data in terms of water sources, evolution and mixing, geochemical equilibria;

- highlight specific sampling or analytical issues, ensuring that highly-ranked samples do not have single deleterious factors or erroneous data that 'slip through' the quality classification system;

- give appropriate relative weights and ranks to problematic data so that causes of unreliability are flagged and also that information is not lost;

- provide valid guidance on the quality of data for isotopes, gases and trace elements, in addition to indicating reliability of general compositional data.

1.3.2 Characteristics required for a scoring system aimed at Tono data

The quality scoring schemes that have been devised previously elsewhere generally focus on the overall 'quality' of the data from a given sample. For example, data from samples that are highly contaminated by drilling fluid are considered to be generally less reliably than data from samples that are less contaminated. The present project aims to go further than this classification by highlighting factors that affect the reliability of data for particular purposes, in addition to highlighting indicators of overall quality. The data quality should be classified relative to a range of benchmarks that corresponds to the range of purposes for which the data will be used.

To reflect this requirement, the approach that is adopted here is not to represent sample quality by numbers on a scale that indicates how 'good' a sample is, but rather to record our degree of belief that it is fit for some purpose. When evaluating whether the data are fit for this purpose, a judgement is made as to whether or not uncertainty in the in-situ water composition estimated from the analytical data would be the greatest cause of uncertainty in the final outcome of a geochemical interpretation (solubility of radionuclides, origin of salinity, residence time of groundwater etc). If the uncertainty in in-situ composition is judged to be less than the other uncertainties associated with an interpretation, then the chemical data are deemed to be of sufficiently high quality. On the other hand, should the uncertainty in the in-situ composition be judged greater than the other uncertainties, then the chemical data would be considered to be of insufficiently high quality. Examples that illustrate this approach are given as follows:

- ▲ The data are deemed to be of sufficiently high quality if an analysed composition is insignificantly different from in-situ composition at that location. Possible definitions of 'insignificant' are that the uncertainties in the data:
  - would be within accepted analytical error of the water;
  - any difference between the analysis and actual water composition would have no impact on a Performance Assessment (PA) or Safety Assessment (SA);
  - any difference between the analysis and the actual water composition would cause radionuclide solubility to vary by less than normally accepted analytical error.
- ▲ The data are deemed to be of sufficiently high quality for distinguishing the origins of salinity if the differences between the analysed compositions and the in-situ compositions of determinands that indicate origins are less than differences between components in different sources. For example, if we use Br/Cl ratios, then the difference between the analysed Br/Cl ratio and the in-situ Br/Cl ratio is less than the difference between the Br/Cl of seawater and the Br/Cl ratio of (say) halite. An implication of this approach is that the data are of sufficiently high quality to allow identification:
  - the origin of some component (i.e. good enough to state the 'there is a component of seawater here')
  - the amount of some component (e.g. we have a water with 25% of seawater)
- ▲ The data are deemed to be of sufficiently high quality for estimating the residence time of groundwater salinity if the difference between the residence time indicator in the water sample and the residence time indicator in-situ are insignificant. In this case, 'insignificant' means that the difference would result in a difference in estimated residence time smaller than the conceptual/theoretical uncertainties associated with the residence time method. For example, to interpret ^{14}C data in terms of residence time requires knowledge of ^{14}C at recharge, dilution of ^{14}C by 'dead' C etc. The uncertainties in these processes cause uncertainties in the estimated residence time. If these uncertainties are greater than the uncertainty that would be caused by the difference between the analysed and in-situ ^{14}C concentration, then the quality of the sample may be judged to be 'good enough'.

JNC's most important need is to evaluate the quality of data from the perspective of PA and SA. Such PA and SA involve calculating the solubility and migration of radionuclides. Therefore it was decided to focus on evaluating the suitability of the geochemical data for estimating the solubility and aqueous speciation of radionuclides. Thus, the quality classification system is aimed primarily at evaluating the quality of geochemical parameters that affect the solubility of radionuclides.

From the results of past sensitivity analyses evaluating solubility (Metcalfe et al., 2004), important geochemical parameters are shown in the left column of Table 1-1. To evaluate the quality of these parameters, the related parameters in the central and right-hand columns are important. In accordance with this work, important evaluation items to judge the quality of geochemical parameters shown in Table 1-2 will be abstracted.

Table 1-1 Relationship between the most PA/SA-relevant parameters and other parameters. The PA/SA-relevant parameters are listed in the first column. However, other parameters would also be evaluated in order to assess the quality of these parameters (colored column). Oxidized and reduced Fe and S would be assessed for consistency with Eh; major cations would be used to evaluate charge balance; TIC and alkalinity would be used to assess the consistency of pH, HCO_3^- and CO_3^{2-}.

Main PA-elevant parameter to be evaluated	**Additional parameters to be considered when evaluating the primary parameter**		
	Fe^{2+}, Fe^{3+}, HS^-	Major cations (Na, K, Ca, Mg)	TIC, Alkalinity
Eh	🟨	🟨	
pH		🟨	🟨
HCO_3^-		🟨	🟨
CO_3^{2-}		🟨	🟨
SO_4^{2-}		🟨	
PO_4^{2-}		🟨	
TOC			

Table 1-2 Groups of parameters to be evaluated.

Groups of parameters to be evaluated
Eh
Oxidized and reduced Fe (Fe^{2+}, Fe^{3+})
Reduced S (HS^-)
pH
Alkalinity
Inorganic carbon species (TIC, HCO_3^-, CO_3^{2-})
Major cations (Na^+, K^+, Ca^{2+}, Mg^{2+})
Major anions (Cl, SO_4^{2-})
PA-relevant trace constituents (PO_4, TOC)

2 Task 1: Review of quality information

2.1 Approach to the review

Task 1 of the project involved reviewing information that is relevant to understanding the quality of groundwater chemical compositions obtained during JNC's past investigations in the Tono area (e.g. DH-, MIU-, MSB- series borehole investigations). At the outset of the project, it was recognised that the the scope of a review would depend partly on the nature of the documentary records available and also on the priorities of JNC. These issues were discussed with JNC at a project start-up meeting on 29th November 2004. Based on this discussion, the following approach was adopted:

- ▲ The quality classification system developed by JNC during 2003 was reviewed, taking into account the latest information about data quality.
- ▲ The borehole report for deep borehole DH-15 was reviewed.
- ▲ Based on the review a plan for assessing the quality of all JNC's boreholes was made.

The decision to focus initially on borehole DH-15 was taken because:

- It is a recently drilled borehole, (final straddle packer test, No. 20, completed in August 2004) and therefore employed the most recent drilling, sampling and analytical methods.

- The methods followed during drilling the borehole have been well-documented.

- The borehole is located close to the site of the MIU construction site.

The review considered not only information connected directly with data quality (residual tracer concentrations and cation and anion equivalent balance etc), but also information from which the quality of analytical data can be judged indirectly (drilling method, sampling method, sampling interval length, time taken between sampling and analysis, convergence with geophysical parameters, cation and anion equivalent balance etc).

2.2 Review of the preliminary classification system

2.2.1 Indicators of quality considered

The preliminary data quality scoring method developed by JNC in 2003 considered the following data quality indicators:

- degree of contamination by drilling water, as indicated by fluorescent dye (typically eosin) added to the drilling fluid;

- cation-anion charge balance;

- delay time between sampling and analysis of unstable determinands: alkalinity, reduced sulphur and ferrous iron;

- sampling container, i.e. whether in a downhole gas-tight vessel or pumped into an open bottle at the surface;

- evidence from pH, EC and Eh stability from time series monitoring;

- length of discrete sampling interval between packers, i.e. the longer the interval, the greater chance there is of mixing of chemically-discrete groundwater flows within the interval;

- ▲ sampling logistics, i.e. whether in a downhole ‘in-situ’ sampler or pumped to the surface (possibly by air-lifting);
- ▲ location where measurement or analyses of physico-chemical parameters, i.e. downhole, surface monitoring (with flow cell where appropriate), or laboratory.

Quality scores were derived from these items according to the following scheme:

１．Drilling fluid contamination（%）

The % drilling fluid contamination was calculated using the amount of tracer present in the sample. The assumptions are that the tracer is conservative (does not break down or react within the borehole or formation) and is not present in the groundwater. Tracer for contamination of groundwater is occupied by drilling fluid. The score was:

$$Score = \frac{1}{\%conta\min ation}$$

However, if the contamination was less than 1%, then the value was always taken as 1. A score of 0 was used when no fluorescent dye was added to the borehole.

２．Charge Balance

Chemical equivalents were calculated from the analysed values and a charge balance was calculated according to:

$$\text{Balance} = 100 \times \frac{\left(\sum \text{cation} - \sum \text{anion}\right)}{\left(\sum \text{cation} + \sum \text{anion}\right)}$$

The score was calculated according to:

$$\text{Score} = \frac{2}{\text{Balance}}$$

However, when the balance was <2% the score was taken to be 1. A balance within 2% was considered to be desirable when the cation concentration was within 3-10 meq/L. Additionally in cases where there were less than 3meq/L cation equivalents, within ±0.2 meq/L was considered to be acceptable. When the concentration was 10meq-800meq/L ± 2︵5% was allowable.

３． Lag time between sampling and analyses

This part of the scoring system takes into account the fact that some determinands (dissolved inorganic C-species, S- species and Fe-species) are relatively unstable during sampling and storage. Consequently, it is necessary to reflect in the scoring system the fact that the quality of data for these components will depend partly upon the time that elapses between sampling and analysis. However, because usually the exact time is not known, quality scores were assigned according to whether the time was < 6 hours, or > 6 hours. If the former, then the time was taken as 6 hours; if the latter, it was taken to be 24 hours. The score was then assigned according to:

$$\text{Score} = \frac{6}{\text{Time}}$$

However, in cases where the duration was greater than 6 hours, but the sample was preserved by using a sampler that kept in-situ conditions（Multi-Piezometer System (MP)) or 1000m sampling device, the lag time was taken to be 6 hours.

４． Sample container

In the case where sampling was done using a sampler that can keep an in-situ atmosphere（MP and 1000m sampling device bottle）the score was taken to be 1. In cases where the sample was transferred to a polythene bottle etc and analysed on the surface, the score was taken to be 2. The score was not used directly in the scoring system, but is simply a flag to indicate the nature of the sample storage container.

５． Stability of pH, EC, Eh

The stability of pH, EC and Eh , as measured using a monitoring device or sampling device were judged. The final values were compared with the values measured 5 hours earlier and the values at one hour intervals within the 5 hour period were evaluated. The score was calculated according to:

$$\text{Score} = \frac{0.2 \times 0.001}{\text{Stability}_{\text{pH}}}$$

$$\text{Score} = \frac{0.2 \times 0.01}{\text{Stability}_{\text{EC}}}$$

$$\text{Score} = \frac{0.2 \times 0.1}{\text{Stability}_{\text{Eh}}}$$

In each case the biggest possible score is taken to be 0.2, reflecting the fact that drilling fluid contamination was judged to always affect the measured values, so that higher quality (larger scores) are unattainable. Each parameter value can become zero, but if the denominator becomes zero calculations cannot be carried out. The smallest variations that can be measured are: pH = 0.01/5; EC = 0.1/5 ; Eh = 1/5. In the case where the value was zero the stabilities are taken to be 1/2 these values（0.001, 0.01, 0.1 respectively).

6． Distance between packers

The degree to which a groundwater sample will represent in-situ conditions at a particular locality in the sub-surface depends partly upon the degree to which mixing between different groundwater bodies has occurred during sampling. In turn, this mixing is likely to depend in part on the length of the borehole section from which water is sampled. The greater the length, the greater is the possibility that chemically different groundwaters from different flowing features (porous matrix, fractures etc) will mix. Thus, it was considered that generally sample quality would have decreased as sampling length increased. This was reflected in the scoring system by:

$$\mathrm{Score} = \frac{0.7}{\mathrm{Length(m)}}$$

When the length was 0.7 m the score attained the largest value of 1. This approach reflected the fact that the smallest test section, in borehole KNA-6, was 0.7m.

7． Sampling Location

The quality of measurements depends partly on the location of where a groundwater sample was collected. A quality weight of 1 was assigned to a sample if it was collected in-situ using a 1000m sampling device, and MP system or other down-hole equipment. In contrast a weight of 2 was assigned if a sample was collected at the surface during a pumping test etc, unless air-lifting was used, in which case the weight was zero. A quality score was then calculated according to:

$$IF\left(Weight = 1OR2, Score = \frac{1}{Weight(1,2)}\right), ELSE(Score = 0)$$

8． Physico-chemical parameter measuring location

The quality of measurements of physico-chemical parameters (Eh, pH, EC, temperature etc) was considered to reflect the locations where measurements were made. When parameters were measured in-situ, they were assigned a quality weight of 1. In contrast, parameters measured in monitoring devices or flow cells etc on the surface were assigned a quality weight of 2. Measurements made in the laboratory were given weights of 3. Then, a quality score was calculated according to:

$$\text{Score} = \frac{1}{\text{Weight}(1,2\text{or}3)}$$

9. Overall quality score

An overall quality score was calculated by summing the scores calculated for the individual quality indicators 1 to 8 above (excluding 4). Apart from the scores used in connection with the stability of pH, EC, Eh the largest score is 1. In contrast, the stabilities of pH, EC, Eh have low weights and the largest score is 0.2.

Boreholes that gave water analyses with scores more than 3 are: DH-4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15、KNA-6、MSB、MIZ-1. The most recent boreholes that used the 1000 m water sampling device gave the highest scores. However, in spite of being very contaminated, the water from DH-9 water gave high scores. It is therefore advisable to modify the scoring system so that the samples from this borehole have lower weights.

Conversely, the score of the water sampled from MSB-4 using the MP system is comparatively low, and reflects the length of the sampling section and the ion balance (JNC analysis). However, the samples were kept in bottles and analysis was done on-site in November 2003. Therefore a higher score is more appropriate, indicating that the quality scoring system should be modified appropriately.

2.2.2 Availabilityof quality information for existing classification scheme

The scheme outlined above was applied to data available to the end of H15. The availability of the information for the above quality indicators is given in Appendix 1. From this appendix the following can be seen:

- The most complete sets of data quality information were available for the most recently completed boreholes.
- Information was available for all the quality indicators in the cases of samples from MSB-2, MSB-4, MIU-4, DH-10, DH-11, DH-12, DH-13, DH-15, and MIZ-1.
- For most samples information about one or more of the quality indicators outlined in Section 2.2.1 is lacking.

- Quality scores are sometimes quite high for samples that are clearly highly contaminated.

- Owing to the fact that the overall quality score is the sum of quality scores for individual quality indicators, high scores for some indicators compensate for poor scores for other indicators.

2.2.3 Limitations of the preliminary classification scheme

The preliminary classification scheme developed by JNC during H15 does indeed give a very general indication of geochemical data quality, in so far as samples with higher scores are of generally higher quality than those with lower scores. However, the classification scheme leads to several important anomalies, whereby samples of demonstrably low quality have high scores and samples that could be of high quality have low scores.

There are five main underlying limitations to the classification scheme:

- The overall quality scores obtained by adding scores for individual quality indicators. Therefore a high score for one quality indicator will tend to compensate for a low score for another indicator.

- In the cases of many samples there are no data for many quality indicators. This lack of information is reflected in a low overall quality score, since these scores are additive. Thus, the scoring system does not distinguish evidence for poor sample quality from no quality evidence.

- Not all available quality indicators are taken into account by the classification scheme. For example, the degree of consistency between geochemical parameters (e.g. between TIC, HCO_3, CO_3 and pH, or between different redox indicators) is not evaluated.

- The quality indicators chosen as a basis for the scheme do not always indicate quality consistently. For example, the length of a borehole test section may correspond to quality, but not always.

- The weights given to different quality indicators are not necessarily a true reflection of the indicators’ impact on quality. It is suggested that too much weight is given in the classification scheme to factors such as delay time, sampling and monitoring logistics that may be important but are not independent factors.

Contamination by drilling fluid is probably the greatest impact on overall sample reliability. It is therefore anomalous that the classification system has scored a sample from DH-11 (132-135 m) at 3.75 although it has 48% contamination. In this case, the low score due to contamination is offset by high scores due to short delay time, pH/EC/Eh monitoring and stability, and to the fact that these were monitored with a downhole tool. This exposes a limitation of employing an additive scoring system in conjunction with the chosen quality indicators.

Another key aspect of data quality is the reliability of Eh measurements. In many cases the high overall scores include contributions from the scores awarded to samples that have had pH/EC/Eh monitored, and are thus justified. However, the preliminary data classification scheme gives an inconsistent picture of the quality of Eh measurements. For example, the sample from 157.5-164 m in DH-12 has a score >3 and low contamination, but the Eh stability is relatively poor. This results in a relatively low score. Furthermore, the stability of Eh is only meaningful if monitoring is done either downhole or in a flow-through device at the surface. For two samples from DH-15 (63.0 to 72.5 mbgl and 84.5 to 97.5 mbgl) it seems that stability is scored even though monitoring seems to have been done in the laboratory. In such cases, the stability score would be meaningless.

Stability of pH measurements is of similar significance to that of Eh, except that it depends on in-situ carbonate speciation and equilibria and the partial pressure of CO_2, PCO_2. Many of these groundwaters from the Tono area have notably low alkalinities and high pH values (ca. 8.0 to 9.5 range). Such solutions might be unstable after sampling due to ingassing of atmospheric CO_2. Samples MIU-4 and MSB-2 are dilute groundwaters and have low alkalinities and pH >9, but they have fairly good stability during pH monitoring and also high scores. Samples DH-8, -9 and –10 are similar.

The conclusion from these considerations of pH and Eh reliabilities, and whether these are adequately reflected in the quality classification system, is that they are of such importance to geochemical interpretation and modelling that they need to be assessed directly as well as via the quality classification scheme. Whether they are representative of in-situ chemistry depends on a wide and varying range of influences and chemical relationships.

Inspection of the Tono data set shows that low quality scores originate primarily from the absence of tracer data with which to quantify drilling fluid contamination. Secondary factors according to the weights given to the scores are lack of pH/EC/Eh monitoring, monitoring and sampling carried out on water pumped to surface rather than downhole, and charge balance. In most of these situations, low scores do not positively indicate unreliable samples and analyses. Instead they often indicate a minor possibility of deviation from in-situ composition relative to the deviation caused by contamination or Eh and/or pH perturbation. Therefore low quality scores are a warning to data users to critically inspect the sampling conditions and data more thoroughly.

Isotopes, dissolved gases and trace elements each have particular sensitivities to sampling logistics, sample handling and analyses. Thus the quality classification scheme is not adequate on its own as an indicator of data reliability. Individual factors have specific effects on data reliability. For example, the sample container must be an air-tight sealed vessel for dissolved gases, i.e. score = 1 only, otherwise data are meaningless. Carbon isotopes ($\delta^{13}C$ and ^{14}C) need relatively large volume samples from a flowing source plus special preservation after sampling for data to have greatest reliability. High pH groundwaters, which are prevalent at Tono, may easily take up CO_2 from the atmosphere and thus contaminate the in-situ compositions.

Tritium (^{3}H) is a particularly sensitive and potentially important data quality indicator. In deep groundwaters it may be a reliable indicator of contamination by drilling water or near-surface water (as was the case for data from the Sellafield site in England; Nirex, 1997). In more shallow groundwaters where nucleogenic ^{3}H may occur naturally, its detection provides an indication of how deep young (<50 y) groundwaters have penetrated. Therefore decisions to sample, analyse and interpret ^{3}H in undisturbed or underground laboratory situations have to be matched by very careful quality control of data. Quality scores on their own would not be adequate for this, and specific indicators of ^{3}H interferences/contamination must be examined alongside the overall quality classification system. The representativeness of ^{3}H may be strongly affected by even 5% contamination in some groundwaters, e.g. those where 'young' drilling water contaminates old groundwater. The relationship between % contamination and ^{3}H content is unclear in the Tono samples, where for example DH-13 (408-442 m) has 21% contamination according to the fluorescent tracer and also has 1.1 TU of ^{3}H; this suggests that drilling water has a rather low ^{3}H content.

There is a more general discrepancy in that several water samples (e.g. DH-5, -6, -7, -8) have low ^{14}C contents indicating old (e.g. >5000 y) groundwaters, which nevertheless have measurable ^{3}H contents. The latter evidence indicates young water contents, i.e. contamination/mixing, but tracer indications of drilling water contamination do not seem to be high enough to account for the ^{3}H. It may be that contamination by in-mixing of shallow, untraced, groundwater within the borehole is being indicated. Thus, integrated interpretation of isotopic and hydrochemical data in this way may give useful evidence of sample quality that would supplement or replace what the quality scores might suggest.

Such an integrated interpretation could be supplemented further by information concerning the temporal and spatial variations of groundwater heads. This additional information could allow a qualitative appraisal to be made of the likelihood of inflow of untraced groundwater into the test section.

The trace element of most immediate interest is uranium (U). Quality scores alone are unlikely to be a direct indication of the reliability of U data, since the factors being considered in the scores are not those directly affecting the quality of U sampling. Although U data from Tono are predominantly very low values (<1 ppb), consistent with reducing conditions, there are several anomalies that are unexplained by the quality rankings. For example, TH-1 and –2 have scores >2, but have high U of 28 and 8 ppb. In DH-6, -7 and − 8 samples, U varies up to 4.4 ppb in samples that also have confirmed highly negative Eh values, i.e. There is not a correlation of U variation with redox variation. This suggests that there may be artefacts in U sampling, for example due to variable amounts of colloidal material passing through filters. As in the previous paragraph, this shows that careful inspection, comparison and interpretation of trace element and other hydrochemical data provides additional insights on data quality.

3 Task 2: Development of Evidence Support Logic (ESL) models

3.1 Introduction to Evidence Support Logic (ESL)

3.1.1 Theory of ESL and parameters used

Evidence Support Logic (ESL) is a framework for building confidence in the dependability of decisions. In the present project, the aim is to decide whether the qualities of geochemical data are adequate for evaluating the solubility of radionuclides. The ESL methodology applied in this work has been developed from one described by researchers at Bristol University, U.K. (Cui and Blockley, 1990; Foley et al., 1997; Hall et al., 1998; Blockley and Godfrey, 2000; Davis and Hall, 2003). The methodology has been adapted by Quintessa (Bowden, 2004), primarily for application in the field of model interpretation. Quintessa has also developed the computer code TESLA (The Evidence Support Logic Application, currently version 1.6; Jackson, 2004) to implement this methodology. This software was used in the present project and the illustrations Figure 3-1, Figure 3-4, Figure 3-5 and Figure 3-6 below are based on TESLA’s Graphical User Interface.

The initial step in an evaluation using ESL is to construct a hierarchy of processes (a process model) to link the main process of interest to data or information, usually via intermediate processes (Figure 3-1). In TESLA's interface any process that supports a process directly (without intermediate processes) is referred to as a 'child node'; conversely, any process that is supported directly by such a 'child node' is called a 'parent node'. Thus, in Figure 3-1 Process I1 is a parent node of the 'child nodes', Processes E1 and E2. Similarly, Process I1 is a child node of Process P and Process P is the parent node of Process I1. Generally, the nodes that are furthest to the right should correspond to qualitative information and/or numerical data, whereas intermediate nodes may correspond to parameter values that are derived from the qualitative information and data.

Here, a 'process' is any judgement of information, such as 'evaluating the quality of pH data'. The 'evidence' for each supporting process (E1 to E4 in Figure 3-1) is the extent to which information leads to confidence in its dependability (i.e. support for the process). The 'evidence' for each process is judged with respect to a criterion for the success of the process. For example, if we are evaluating the quality of pH data, then the criterion for success might be 'The measured pH differs insignificantly from in-situ pH'. It is necessary to define each criterion precisely in order to maximise objectivity. In this example the meaning of 'differs insignificantly' needs to be stated clearly. One possibility would be to state that a difference between measured and in-situ pH is insignificant if it would cause a variation in the solubility of a radionuclide that is less than the analytical error on a direct solubility measurement.

In practice evidence for and against the dependability of a process are considered independently (though considering the same criteria for success). For example, one of the processes that must be carried out to evaluate the quality of pH data might be 'Evaluating drilling fluid contamination'. The criterion for success might be that the drilling fluid contamination is insignificant, where 'insignificant' is defined as above. In this case, evidence for drilling fluid contamination being insignificant might be that drilling fluid tracer concentrations are effectively zero. Evidence that the process will fail (that is drilling fluid contamination is not insignificant) might be that alkali drilling fluid additives were employed, so that pH would not vary linearly during mixing.

Once determined, the evidence furthest to the right is then propagated through the process model so as to estimate the reliability of the process of interest (P in Figure 3-1).

To represent evidence and propagate the uncertainties, ESL uses Interval Probability Theory. This theory allows statements of the type: 'The degree of confidence that evidence supports the proposition lies between p and p+u'. Here, p is the minimum

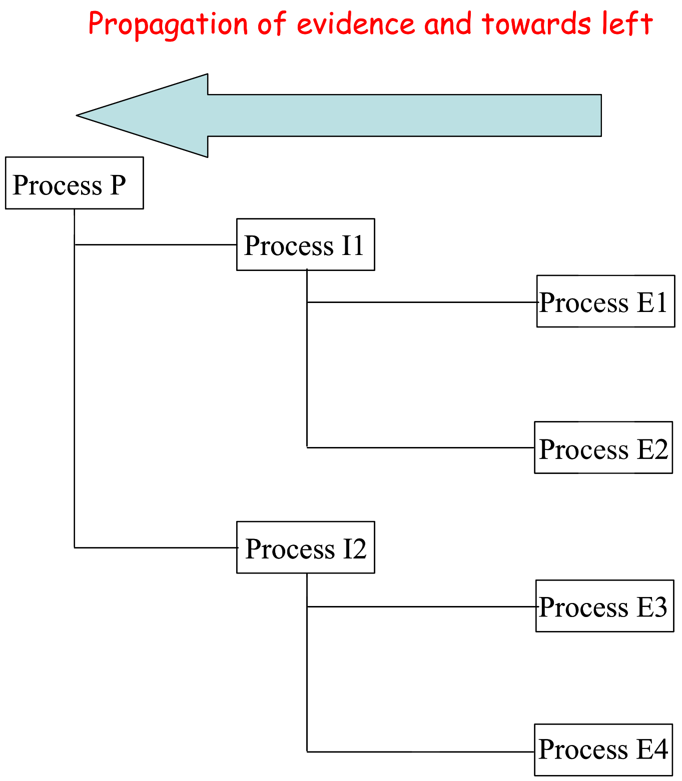


Figure 3-1 A simple ESL process model. The main process of interest, P, is linked to processes E1 E2, E3 and E4 via intermediate Process I1 and I2. Evidence for the success of Processes E1 and E2 supports Process I1, whereas evidence against the success of Processes E1 and E2 refutes Process I1. Similar relationships exist between Processes E3 and E4 and Process I2. See text for explanations of Processes and evidence.

probability that evidence supports a proposition and u is the uncertainty in this probability. The minimum degree of confidence that some evidence does not support the proposition is 1-p-u. In contrast, the classical (point) probability theory requires that if evidence supports a proposition with probability p, then the probability against the proposition is automatically 1-p (Figure 3-2).

Therefore, an advantage of ESL, as applied to the evaluation of groundwater chemical data quality, is that it distinguishes cases where the quality of data is poor, from cases where the quality of the data is simply unknown.

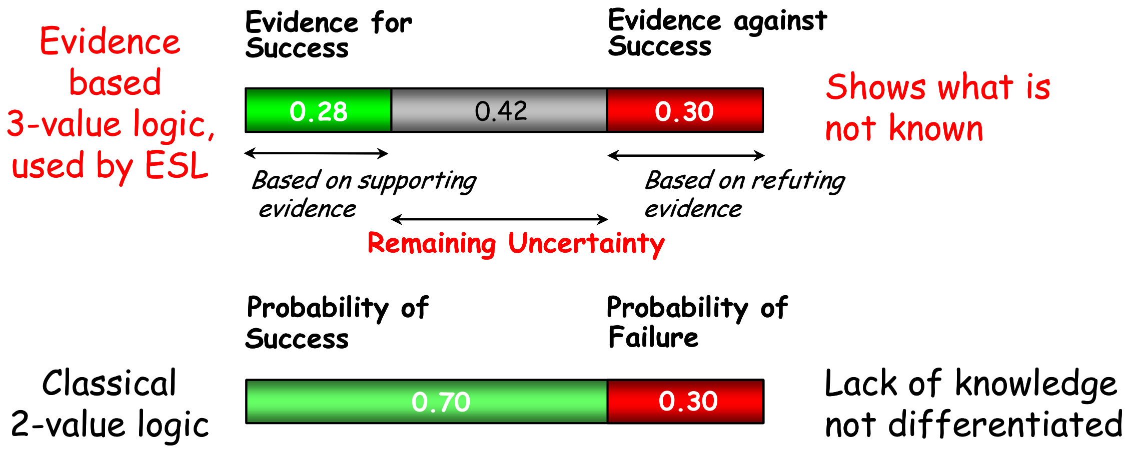


Figure 3-2 Comparison between the approach to treating evidence adopted by ESL (above) with that adopted by the classical approach (below).

The parameters 'sufficiency' and 'dependency' are used to propagate the 'evidence for' and 'evidence against' each process through a process model (Figure 3-3 and Figure 3-4). The 'sufficiency' of an individual piece of evidence or supporting proposition can be regarded as the corresponding conditional probability. That is, the 'sufficiency' of some process as support for another process, is the probability of the latter proposition being true when the supporting proposition is true, irrespective of whether the other processes are true or false.

The user of TESLA also has the option of specifying that all of a set of child nodes must be successful in order for the parent to be successful. Alternatively, the user could specify that the success of any one of a set of child nodes would be sufficient for the success of the parent. These options are illustrated in Figure 3-5.

If a process must be successful in order for the parent process to be successful, then a boolean operator termed 'necessity' is used in place of 'sufficiency'. This parameter changes how the evidence is propagated (Figure 3-1).

A parameter called 'dependency' represents the degree of overlap in the sources of the evidence for the process. This parameter is introduced to avoid double counting of support from any mutually dependent pieces of evidence (Figure 3-3).

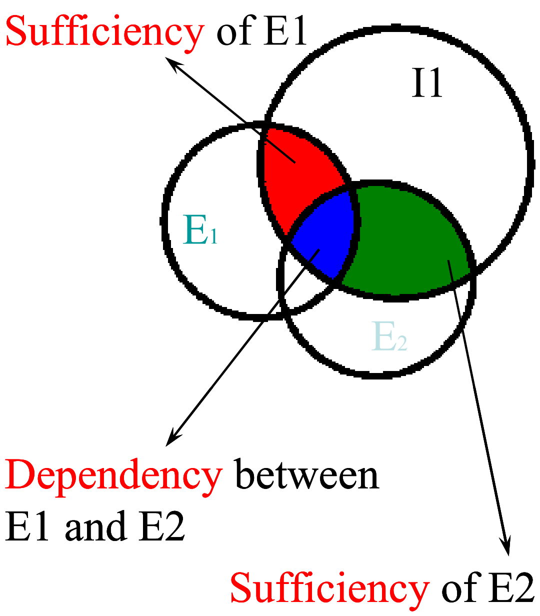
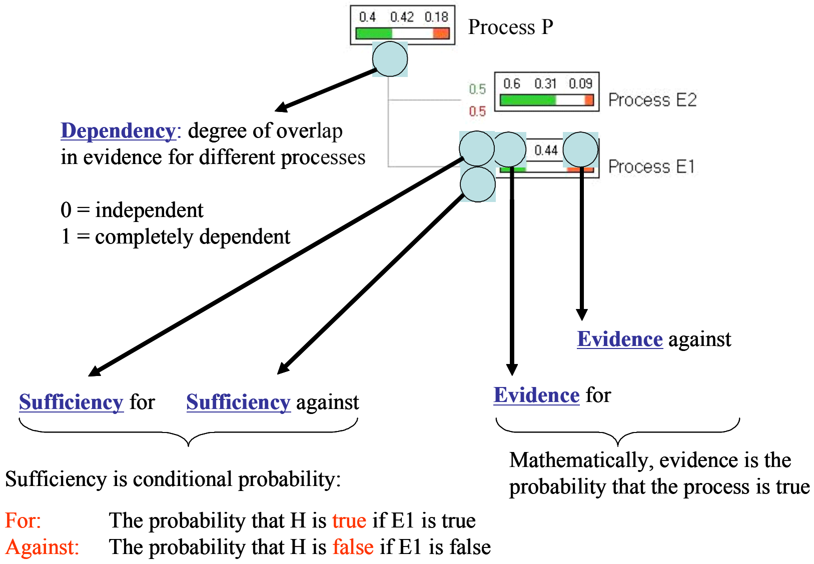


Figure 3-3 Schematic illustration of the parameters sufficiency and dependency. The support provided by Process E1 for Process I1 is represented by the red+blue areas. The support provided by Process E2 for Process I1 is represented by the green+blue areas. The propagation arithmetic must count the blue area only once.



Dependency: degree of overlap in evidence for different processes

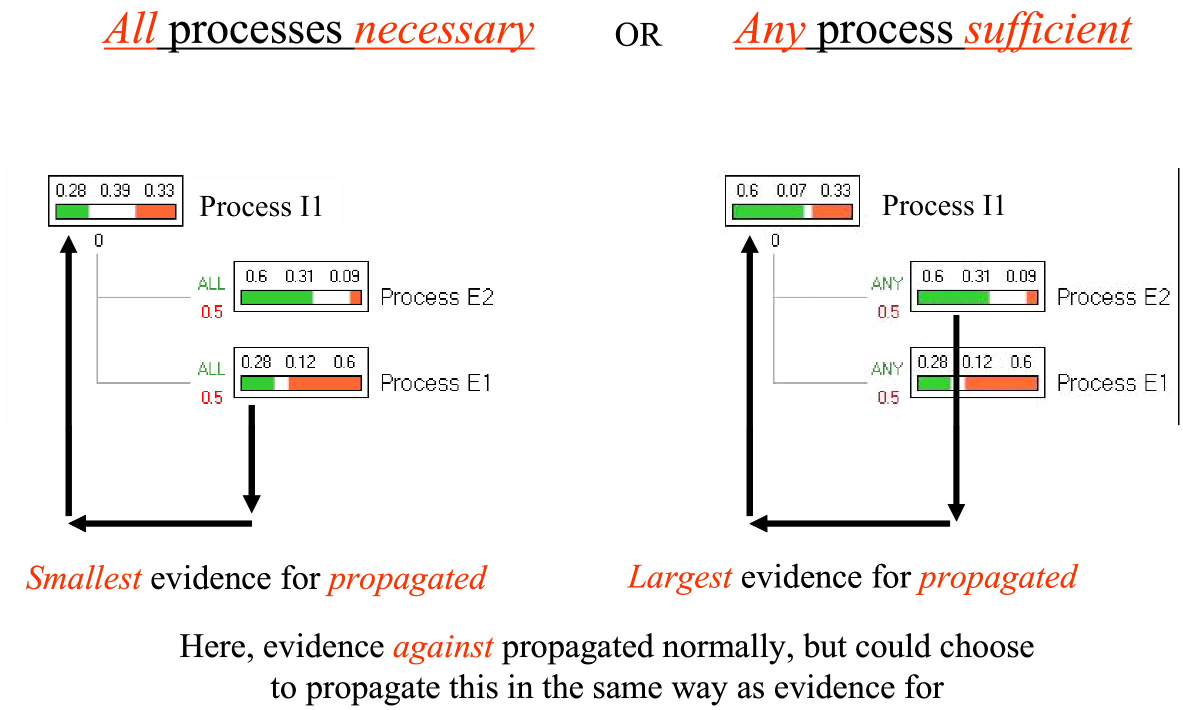
0 = independent
1 = completely dependent

Sufficiency is conditional probability:

For: The probability that H is true if E1 is true
Against: The probability that H is false if E1 is false

Mathematically, evidence is the probability that the process is true

Figure 3-4 Illustration of the sufficiency and dependency parameters used to propagate evidence for and against each process, as they appear TESLA's interface.

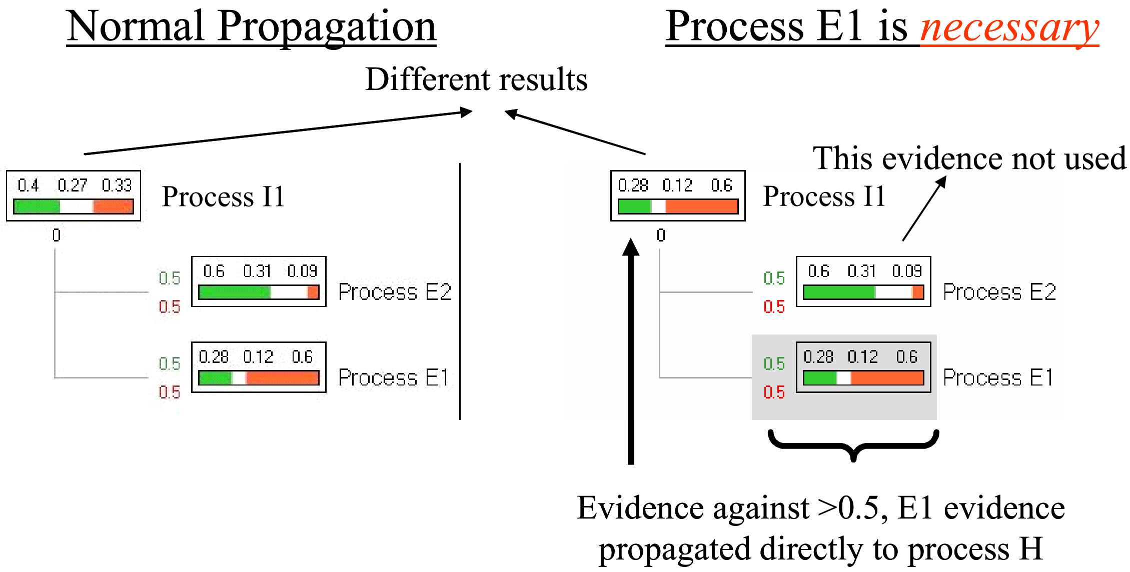


All processes *necessary* OR *Any* process *sufficient*

Smallest evidence for *propagated* *Largest* evidence for *propagated*

Here, evidence *against* propagated normally, but could choose to propagate this in the same way as evidence for

Figure 3-5 Illustration of how the options 'All' or 'Any' change the way in which evidence is propagated through a process model.



Normal Propagation Process E1 is *necessary*

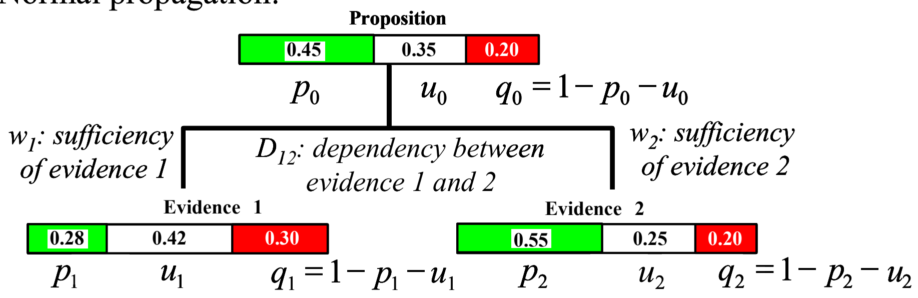
Different results

This evidence not used

Evidence against >0.5, E1 evidence propagated directly to process H

Figure 3-6 Schematic illustration of the effect of the 'necessity' operator. Using the values for the parameters sufficiency (including necessity) and dependency, the evidence for and against each supporting process is propagated through the process model, using the arithmetical procedure illustrated in Figure 3-7.

Normal propagation:



$$p_0 = w_1 p_1 + w_2 p_2 - \rho_{12} Min(w_1 p_1, w_2 p_2)$$

$$q_0 = w_1 q_1 + w_2 q_2 - \rho_{12} Min(w_1 p_1, w_2 p_2)$$

Where:

$$\rho_{12} = \frac{(1 - D_{12})(w_1 p_1 w_2 p_2)}{Min(w_1 p_1, w_2 p_2)} + D_{12}$$

Figure 3-7 Illustration of the arithmetic used for propating evidence through a process model.

3.1.2 Approaches to using ESL

Previous applications of ESL have focussed on developing consensus opinions as to the validity of some proposition (e.g. Seo et al. 2004; Okubo et al. 2004). The general approach has been to capture the opinions of a group of experts. There are several approaches by which this might be achieved, depending upon the nature of the information, the numbers of the experts and their specialities. The simplest approach is for a single person acting as a facilitator to lead the construction of a process model in a meeting involving the experts. At each stage, the structure can then be debated until a consensus is reached. However, the approach to using ESL in the present project is somewhat different for the following reasons:

- Unlike many other applications of ESL, where the success of the main proposition being evaluated (i.e. proposition P in the Figure 3-1 and Figure 3-4) is not subjective, the application of ESL to evaluate geochemical data quality involves considerable subjectivity in the main proposition being evaluated. For example, if ESL is applied to evaluate the proposition that a dam will be safe, there may be little argument about the criteria for success; the dam will not fail. However, the proposition that geochemical data are of high quality is more subjective.

- When developing a system for classifying geochemical data quality arguably the most important requirement is to record the logic used and to ensure that it can be applied as objectively as possible by later users of the system. That is, ESL is used to
    - audit sampling, storage and analytical methodologies;
    - record quality information;
    - clearly record the logic underlying the quality classification system.

3.2 Processes to be considered

The processes to be included in the process models must be related to indicators of data quality. In addition to the quality indicators considered by the scheme developed by JNC in H15 (Section 2.2.1), other general quality indicators that might be considered include:

- consistency of determinations of pH, TIC, alkalinity, HCO_3, CO_3;
- internal consistency of redox indicators (e.g. CH_4 in samples with reducing Eh);
- completeness of an analysis;
- natural tracers for 'young' groundwater samples, indicating contamination by natural water drawn in to the test section;
- appearance of 'odd' chemistry – i.e. chemistry that would not generally be expected in natural waters in this kind of setting;
- amount of water pumped before sampling;
- characteristics of borehole completion (e.g. whether cemented or not);
- information about characteristics of drilling equipment (steel, stainless etc);
- details of remedial measures to rectify borehole stability (e.g. use of LCM, cementing etc);
- information about cleaning of borehole walls (e.g. use of acid fluids to remove drilling fluid cake);
- evidence for correct functioning of sampling equipment (no packer leakage etc);

- characteristics of transfer of samples from sample bottles to analytical equipment (e.g. aerobically, anaerobically);
- information about sample preservation (e.g. filtration, acidification etc);
- information about characteristics of sample storage (e.g. storage vessels, storage conditions);
- consistency of analysed duplicates.

Some of the general quality items correspond directly to reported data. For example, the degree of drilling fluid contamination corresponds closely to measurements of drilling fluid tracers. However, most of these general quality indicators depend in turn on other processes. That is, sub-process models could be constructed to evaluate most of these quality indicators, linking each general quality indicator to actual observations and analytical results. By developing such links to specific data items the final overall process model becomes easier to use objectively as a data quality classification tool.

3.3 Draft ESL process models

3.3.1 Approach to process model development

For the reasons given in Section 3.1.2 , the present project did not aim to develop a consensus among a large group of experts as to data quality. Instead the following approach was adopted:

- Quintessa developed an initial data quality classification system in consultation with JNC.
- The initial data quality classification system was then reviewed by Dr A.H. Bath of Intellisci Ltd, U.K.. Dr Bath is an expert on the interpretation of groundwater chemical data, with experience in many site investigations connected with the geological disposal of radioactive wastes.
- Based on the review comments, the initial quality classification scheme was refined. The main emphasis was to ensure a practical system (not overly complex) which nevertheless takes into account all the major processes that might affect data quality.

In general no unique process model can be constructed to evaluate any particular proposition. Instead, more than one model, each with a different structure, could be developed to address different a particular issue. Usually, each model will contain the same, or very similar processes, but the sufficiencies assigned to the same process will be different in different models. This approach reflects the fact that in different models a particular process will be connected to (give support to) different processes at the next level to the left.

The structure of a process model will depend upon:

- the perspective(s) of the person or people who construct the model;
- the desirability of simplifying a model;
- the need to ensure as far as possible that the model reflects known relationships between different processes in the real world (that is, the requirement to ensure that sufficiencies can be defined as robustly as possible);
- the need to minimise overlaps (dependence) between different sub-process models.

For example, alternative general model structures that might be used to evaluate the quality of a pH determination for a groundwater sample are given in Figure 3-8 and Figure 3-9.

In the case of the model shown in Figure 3-8, the structure reflects the nature of the information from which quality may be judged, rather than the processes that actually affect data quality. A consequence is that the criterion for the success of each process is less clearly related to the quality of the geochemical data being evaluated. For example, the criterion for success of the process ‘Charge balance is acceptable’ may be that the the charge balance is within ±5%. However, the significance of this range for the quality of pH measurements, which is represented by the left-most process in Figure 3-8 is unclear. This uncertainty is reflected in the low sufficienies of 0.3, for and against this process.

For this reason, the initial process model sent to Dr Bath for review adopted the structure shown in Figure 3-9.

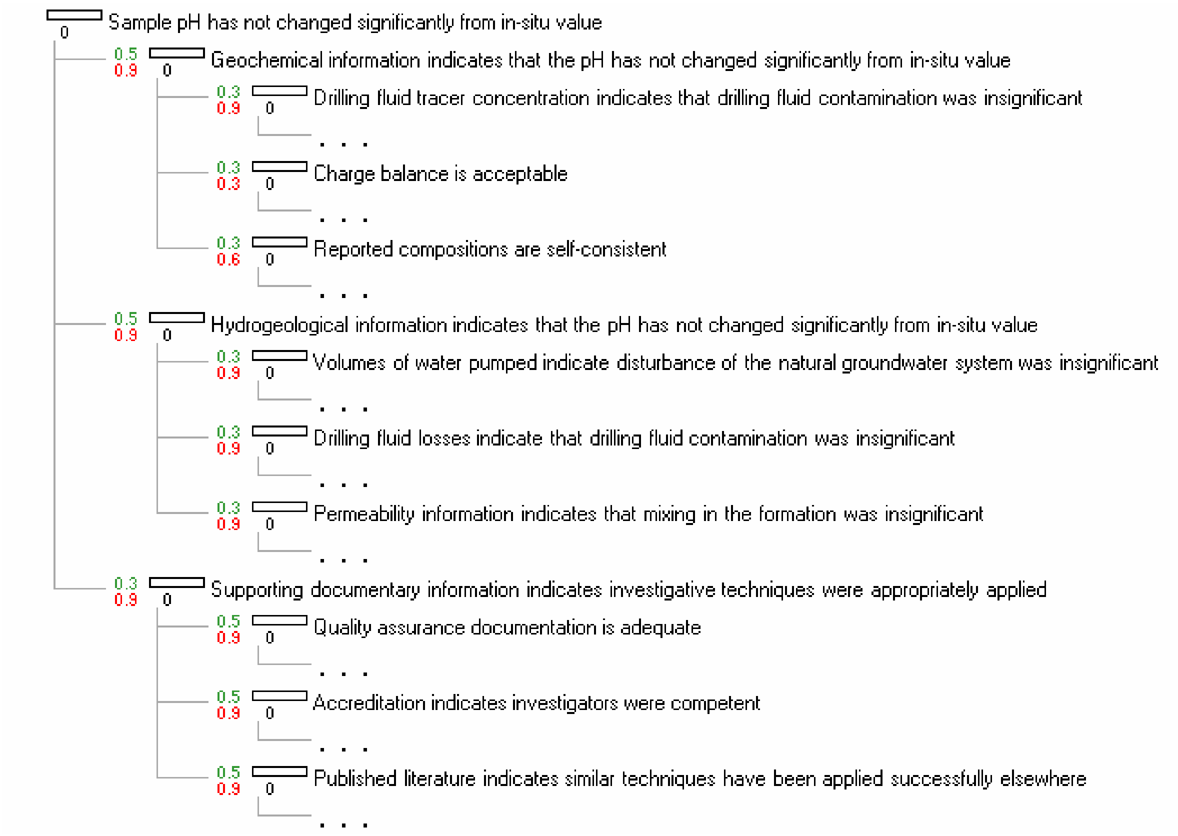


Figure 3-8 An example ESL process model that could be used for evaluating the quality of pH data. The structure reflects the types of information that are available, rather than the physical and chemical processes that affect quality (c.f. Figure 3-9).

Figure 3-9 lternative outline process model showing the overall evaluation of data quality. Processes that have associated sub-process models are indicated by '…' .

The quality of the parameters in Table 1-1 and Table 1-2 will to some extent be affected mostly by the same processes. However different processes will affect different parameters to different degrees. For example, contamination by atmospheric oxygen will be very significant for Eh, but will be much less significant for SO_4. For this reason, it was decided to develop a basic process model for one parameter (pH) initially, and then to modify this for application to other parameters following the review. The chief differences between the models used for different groups of parameters are:

- the sufficiencies assigned to a particular process in different models;

- the criteria used to judge 'success' of each process (e.g. a higher level of drilling fluid contamination is permissible if pH is being evaluated than if Eh is being assessed).

In the present work it was important that initially all processes that might possibly have affected data quality were evaluated. By carrying out such an evaluation the quality information could be audited. Additionally the results can be used to demonstrate clearly to interested parties (peer reviewers, regulators etc) that data quality has been considered thoroughly. However, the process models that represent all of these processes are inevitably highly complex and impractical to use directly as tools for the routine classification of geochemical data according to its quality. Therefore, in practice such a process model must be simplified.

The approach adopted was to initially develop a model that included as many processes as possible. These processes were then compared with the available data quality information to establish:

- whether information with which the success or failure of the processes might be judged actually exist;

- whether these processes are likely to be important for the main proposition that the data are of sufficiently high quality;

- the degree to which the processes will apply to all samples.

Based on this evaluation simplified process models that may be applied to the actual classification of geochemical data according to quality are developed. There were several approaches for achieving this:

- Processes corresponding to quality information that is never available were omitted from the final process models and the values of sufficiency parameters of the remaining processes were adjusted accordingly. This approach ensures that the lack of information is encompassed by the residual uncertainty (the white areas in Figure 3-4, Figure 3-5, Figure 3-6 and Figure 3-7).

- Processes that have little impact on the overall judgement of data quality in practice were omitted from the final process models.

- Different versions of the process models were developed for application to specific sub-groups of samples.

This approach resulted in the initial draft process model illustrated in Figure 3-10.

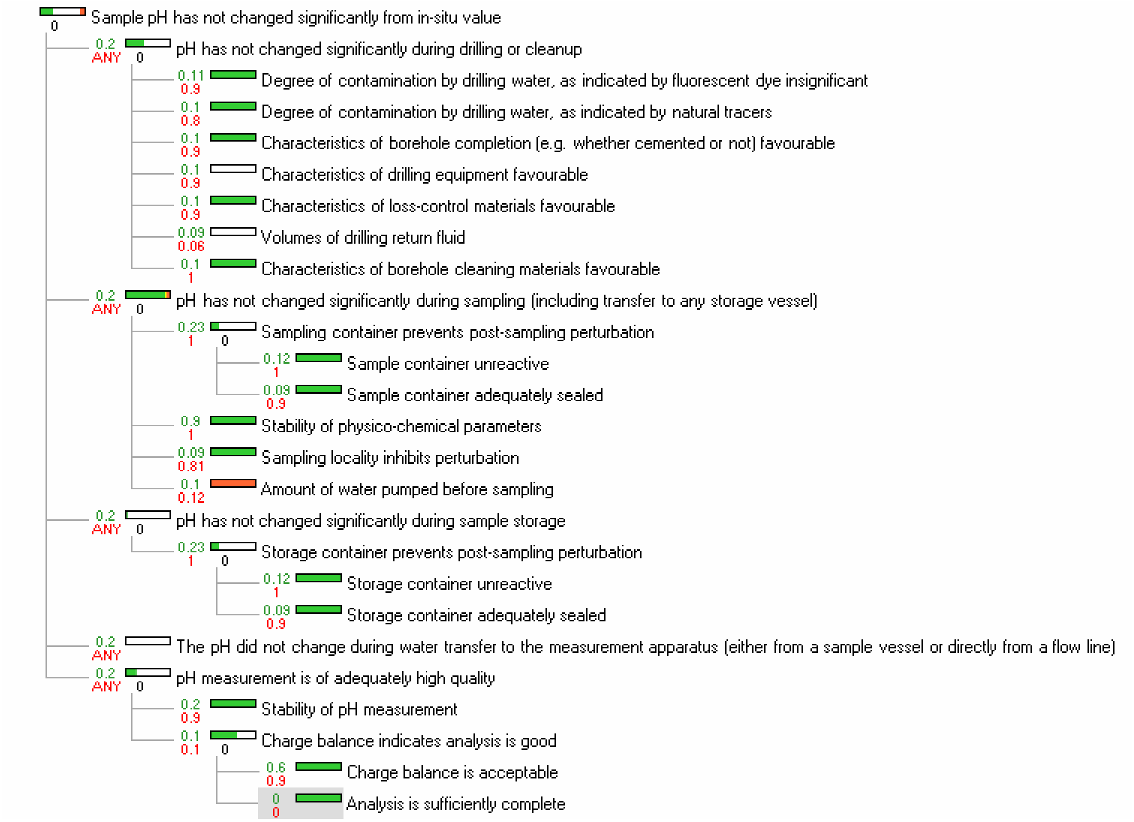


Figure 3-10 Example process model that includes only processes that correspond to possible quality indicators for which information actually exists.

This 'overall' process model and the more detailed process models that underlie it were sent to Dr Bath for review. The models are given in Appendix 2 and Dr Bath's review comments are given in Appendix 3.

3.3.2 Revised process models

Based on the review comments, the draft models were revised as follows:

- Drilling fluid contamination is clearly separated from other processes. The sufficiencies assigned are such that drilling fluid contamination must be below a specified value for quality of the evaluated measurement to be deemed adequate.

- Quality indicators that are distinct from drilling fluid contamination are evaluated separately and are divided into two groups:

  - processes related to analytical evidence indicating data quality (which can be evaluated against clear numerical criteria);
  - processes that indirectly indicate data quality.

- Processes that indirectly indicate data quality are either:
  - processes that rely on other information (i.e. sub-models could be constructed to the right of these processes in the models);
  - processes that are not necessarily clearly related to quality (e.g. discolouration of a sample suggests that the measured pH may not be adequate, though this is not necessarily the case).

It was decided that, rather than develop a separate process model for each group of parameters in Table 1-2, only four main process models would be devised:

- a process model evaluating pH (which is also be appropriate for the major cations (Na^+, K^+, Ca^{2+}, Mg^{2+}), major anions (Cl, SO_4^{2-}) and PA-relevant trace constituents (PO_4, TOC);
- a process model evaluating Eh;
- a process model evaluating redox-sensitive constituents (oxidized and reduced Fe (Fe^{2+}, Fe^{3+}), reduced S (HS^-));
- a process model evaluating the inorganic carbon system (TIC, HCO_3, CO_3).

An example of a revised process model for evaluating pH information is given in Figure 3-11.

The revised model attempts to make a compromise between being sufficiently comprehensive (taking into account all the main processes that might affect quality) and yet not too complex and impractical. Most of the processes in the lower part of the model (beneath the process 'Indirect evidence indicates that pH has not changed significantly from the in-situ value') could be expanded so that further, more detailed sub-process models occur to the right of the diagram.

The other process models are based upon this one for pH. They are illustrated in Figure 3-12, Figure 3-13 and Figure 3-14. It should be noted that the same processes appear in all the models, even where they are not relevant for the quality of the parameter being evaluated. In these cases, the sufficiencies are assigned zero values, effectively 'switching off' that particular quality indicator. The purpose of retaining such 'redundant' processes is two-fold:

- By retaining the same processes in the different models, the different importance of a particular quality indicator for different parameters can be appreciated.

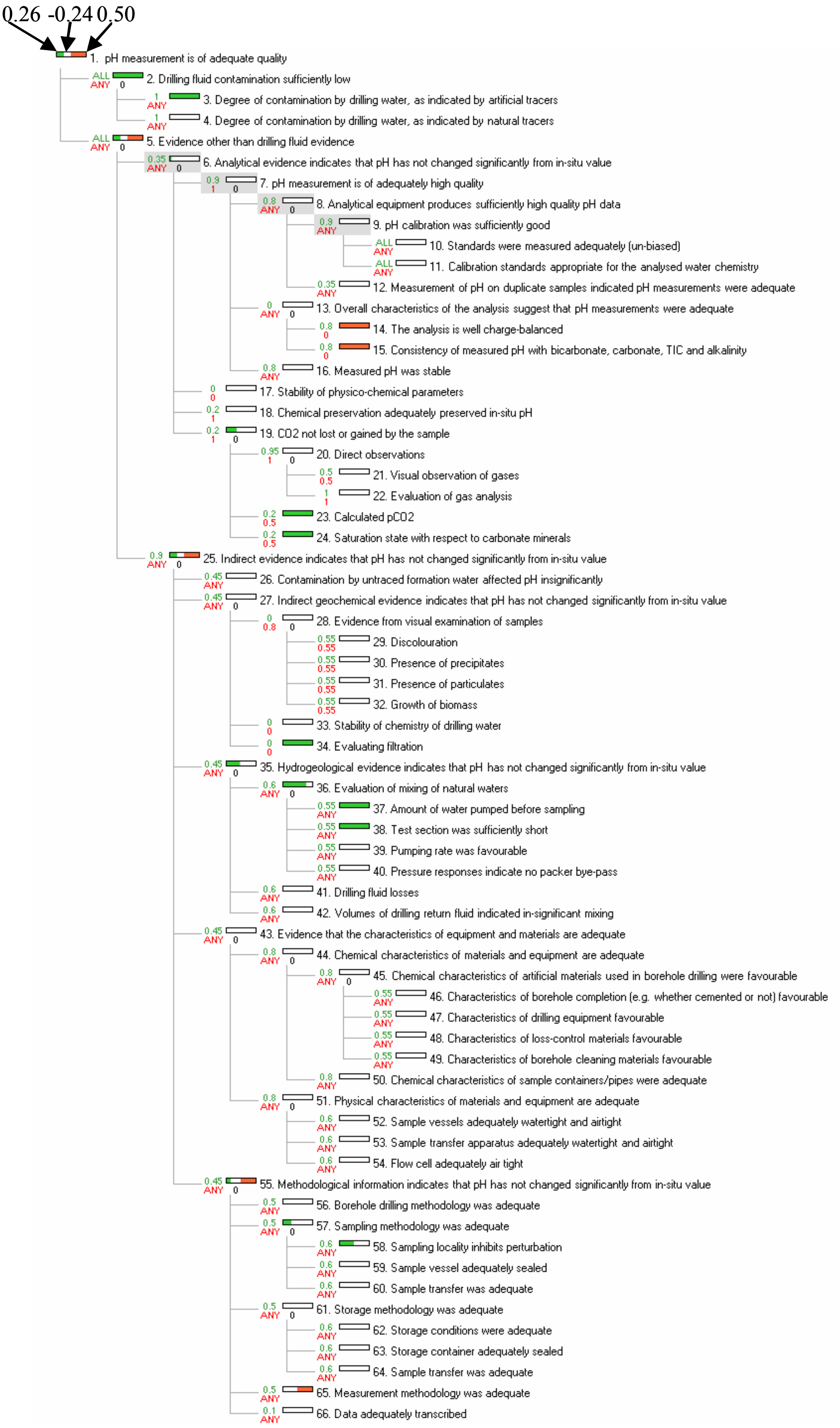
- It is beneficial to record as much quality information as possible, since it enables the user to gain an impression of overall sample quality, which may be relevant to making subjective quality judgements concerning particular parameters.

In the case of the process model evaluating Eh, Process 58 (Sampling locality inhibits perturbation) has been moved to the top and given a much higher weighting. In this case, if the Eh has not been measured in a surface flow-through cell or down-hole, its quality is taken to be inadequate.

The example process models in Figure 3-11, Figure 3-12, Figure 3-12, and Figure 3-13 illustrate several important features of the classification scheme.

- In all the process models in Figure 3-11, Figure 3-12, Figure 3-13, Figure 3-14, there are many processes for which information was unavailable. These appear un-coloured (white). Knowledge that this information is lacking is useful to any interpreter of the analytical data since it helps to convey an overall impression of sample quality.

- In Figure 3-11 a poor charge balance gives rise to evidence against of 1 for Process 14. Similarly, inconsistency between the reported pH, TIC and alkalinity also give evidence against of 1 for Process 15. However, these processes do not contribute to the overall judgement that the pH measurement is of adequately high quality. Instead, the information ‘flags’ potential problems with the overall analysis to the interpreter of the data.



1. pH measurement is of adequate quality
ALL ANY 0 2. Drilling fluid contamination sufficiently low
1 ANY 3. Degree of contamination by drilling water, as indicated by artificial tracers
1 ANY 4. Degree of contamination by drilling water, as indicated by natural tracers
ALL ANY 0 5. Evidence other than drilling fluid evidence
0.35 ANY 0 6. Analytical evidence indicates that pH has not changed significantly from in-situ value
0.9 1 0 7. pH measurement is of adequately high quality
0.8 ANY 0 8. Analytical equipment produces sufficiently high quality pH data
0.9 ANY 9. pH calibration was sufficiently good
ALL ANY 10. Standards were measured adequately (un-biased)
ALL ANY 11. Calibration standards appropriate for the analysed water chemistry
0.35 ANY 12. Measurement of pH on duplicate samples indicated pH measurements were adequate
0 ANY 0 13. Overall characteristics of the analysis suggest that pH measurements were adequate
0.8 0 14. The analysis is well charge-balanced
0.8 0 15. Consistency of measured pH with bicarbonate, carbonate, TIC and alkalinity
0.8 ANY 16. Measured pH was stable
0 0 17. Stability of physico-chemical parameters
0.2 1 18. Chemical preservation adequately preserved in-situ pH
0.2 1 0 19. CO2 not lost or gained by the sample
0.95 1 0 20. Direct observations
0.5 0.5 21. Visual observation of gases
1 1 22. Evaluation of gas analysis
0.2 0.5 23. Calculated pCO2
0.2 0.5 24. Saturation state with respect to carbonate minerals
0.9 ANY 0 25. Indirect evidence indicates that pH has not changed significantly from in-situ value
0.45 ANY 26. Contamination by untraced formation water affected pH insignificantly
0.45 ANY 0 27. Indirect geochemical evidence indicates that pH has not changed significantly from in-situ value
0 0.8 0 28. Evidence from visual examination of samples
0.55 0.55 29. Discolouration
0.55 0.55 30. Presence of precipitates
0.55 0.55 31. Presence of particulates
0.55 0.55 32. Growth of biomass
0 0 33. Stability of chemistry of drilling water
0 0 34. Evaluating filtration
0.45 ANY 0 35. Hydrogeological evidence indicates that pH has not changed significantly from in-situ value
0.6 ANY 0 36. Evaluation of mixing of natural waters
0.55 ANY 37. Amount of water pumped before sampling
0.55 ANY 38. Test section was sufficiently short
0.55 ANY 39. Pumping rate was favourable
0.55 ANY 40. Pressure responses indicate no packer bye-pass
0.6 ANY 41. Drilling fluid losses
0.6 ANY 42. Volumes of drilling return fluid indicated in-significant mixing
0.45 ANY 0 43. Evidence that the characteristics of equipment and materials are adequate
0.8 ANY 0 44. Chemical characteristics of materials and equipment are adequate
0.8 ANY 0 45. Chemical characteristics of artificial materials used in borehole drilling were favourable
0.55 ANY 46. Characteristics of borehole completion (e.g. whether cemented or not) favourable
0.55 ANY 47. Characteristics of drilling equipment favourable
0.55 ANY 48. Characteristics of loss-control materials favourable
0.55 ANY 49. Characteristics of borehole cleaning materials favourable
0.8 ANY 50. Chemical characteristics of sample containers/pipes were adequate
0.8 ANY 0 51. Physical characteristics of materials and equipment are adequate
0.6 ANY 52. Sample vessels adequately watertight and airtight
0.6 ANY 53. Sample transfer apparatus adequately watertight and airtight
0.6 ANY 54. Flow cell adequately air tight
0.45 ANY 0 55. Methodological information indicates that pH has not changed significantly from in-situ value
0.5 ANY 56. Borehole drilling methodology was adequate
0.5 ANY 0 57. Sampling methodology was adequate
0.6 ANY 58. Sampling locality inhibits perturbation
0.6 ANY 59. Sample vessel adequately sealed
0.6 ANY 60. Sample transfer was adequate
0.5 ANY 0 61. Storage methodology was adequate
0.6 ANY 62. Storage conditions were adequate
0.6 ANY 63. Storage container adequately sealed
0.6 ANY 64. Sample transfer was adequate
0.5 ANY 65. Measurement methodology was adequate
0.1 ANY 66. Data adequately transcribed

Figure 3-11 Example of a revised process model evaluating the pH reported for a sample from between 15.8 m and 25.7 m depth in borehole MSB-4. In order to show the model on one page, evidence values are given only for the top level process. 'Evidence for' and 'Evidence against' are overlap (shown in yellow).

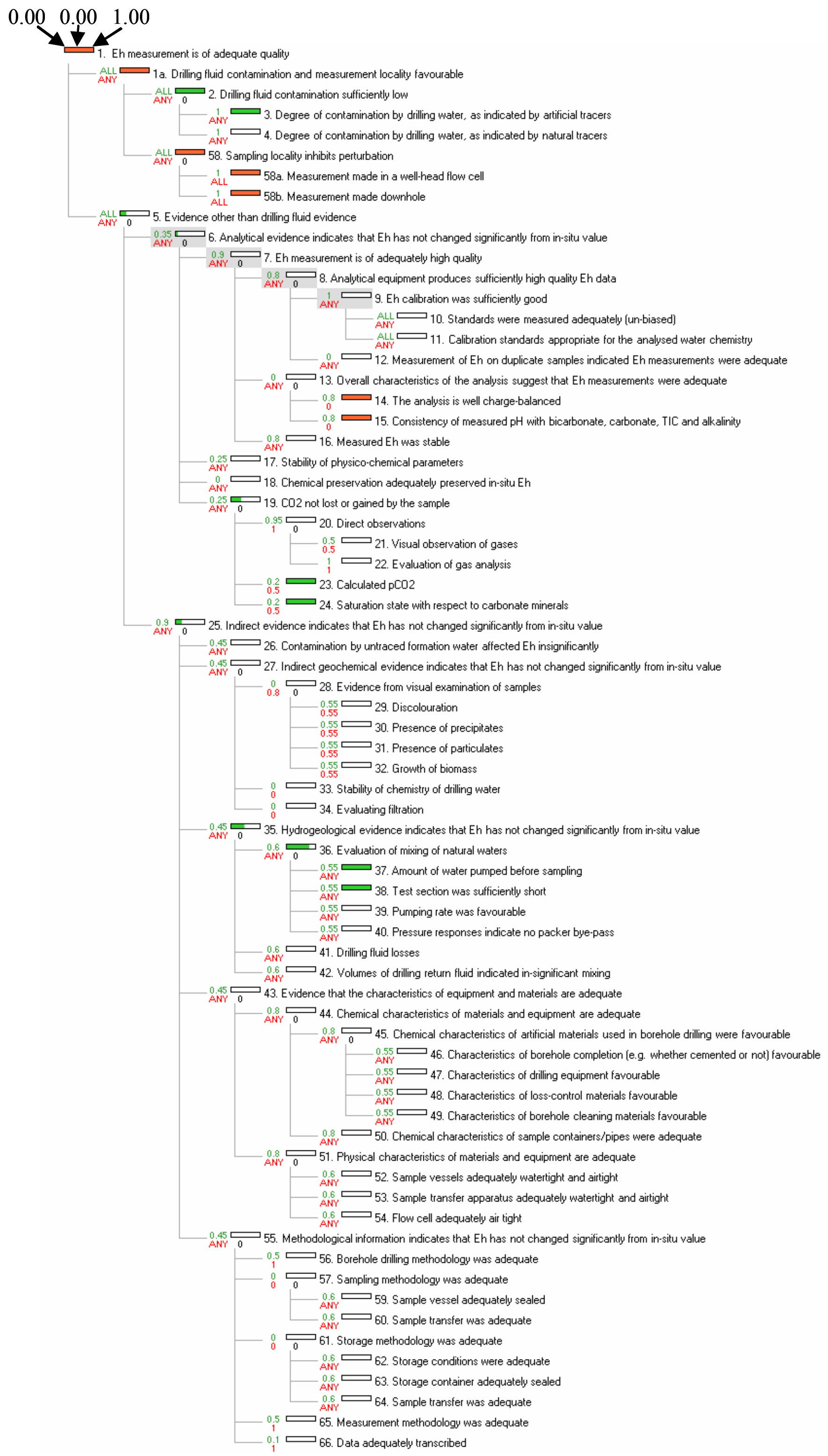


Figure 3-12 Example of a revised process model evaluating the Eh reported for a sample from between 15.8 m and 25.7 m depth in borehole MSB-4. In order to show the model on one page, evidence values are given only for the top level process.

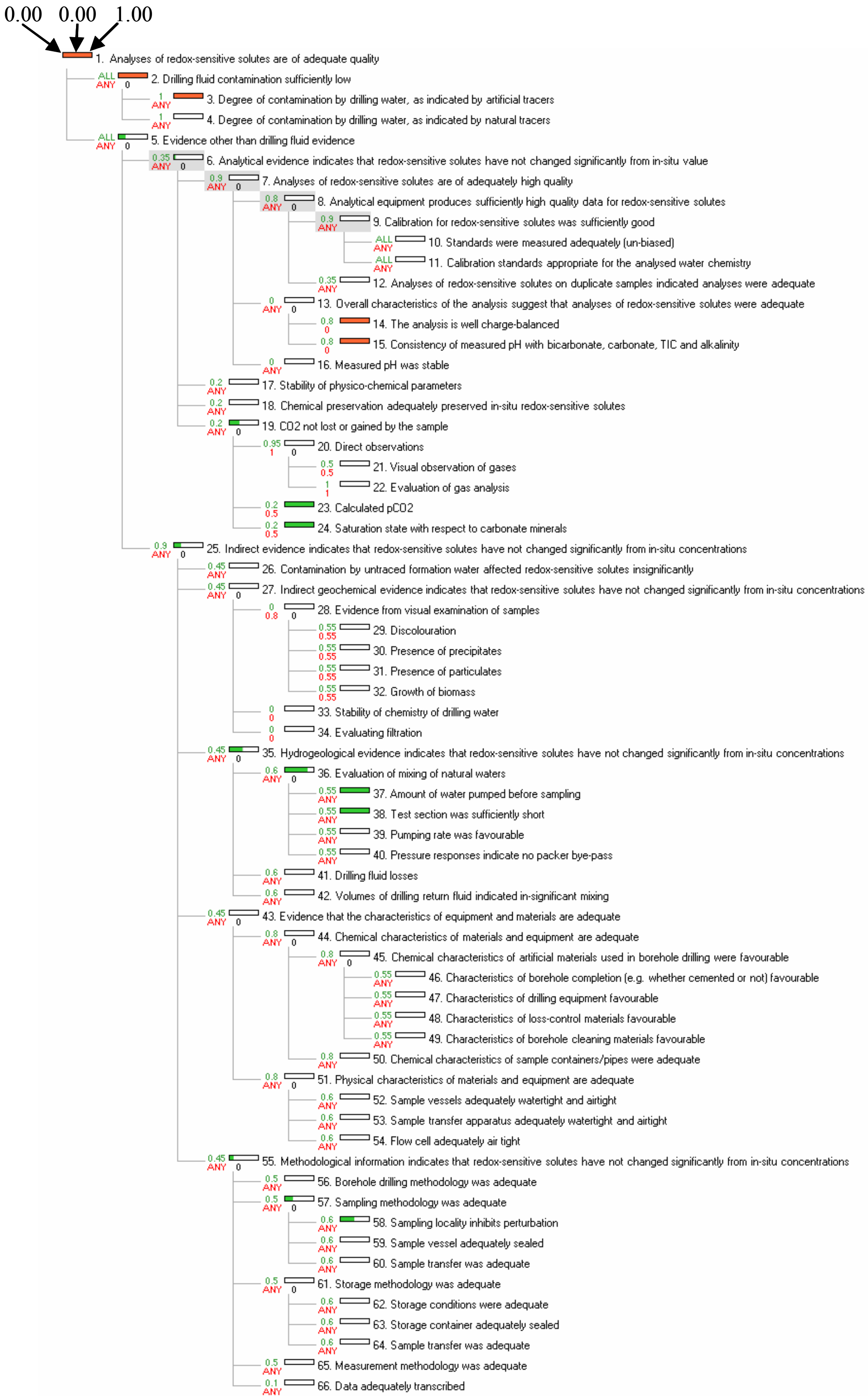
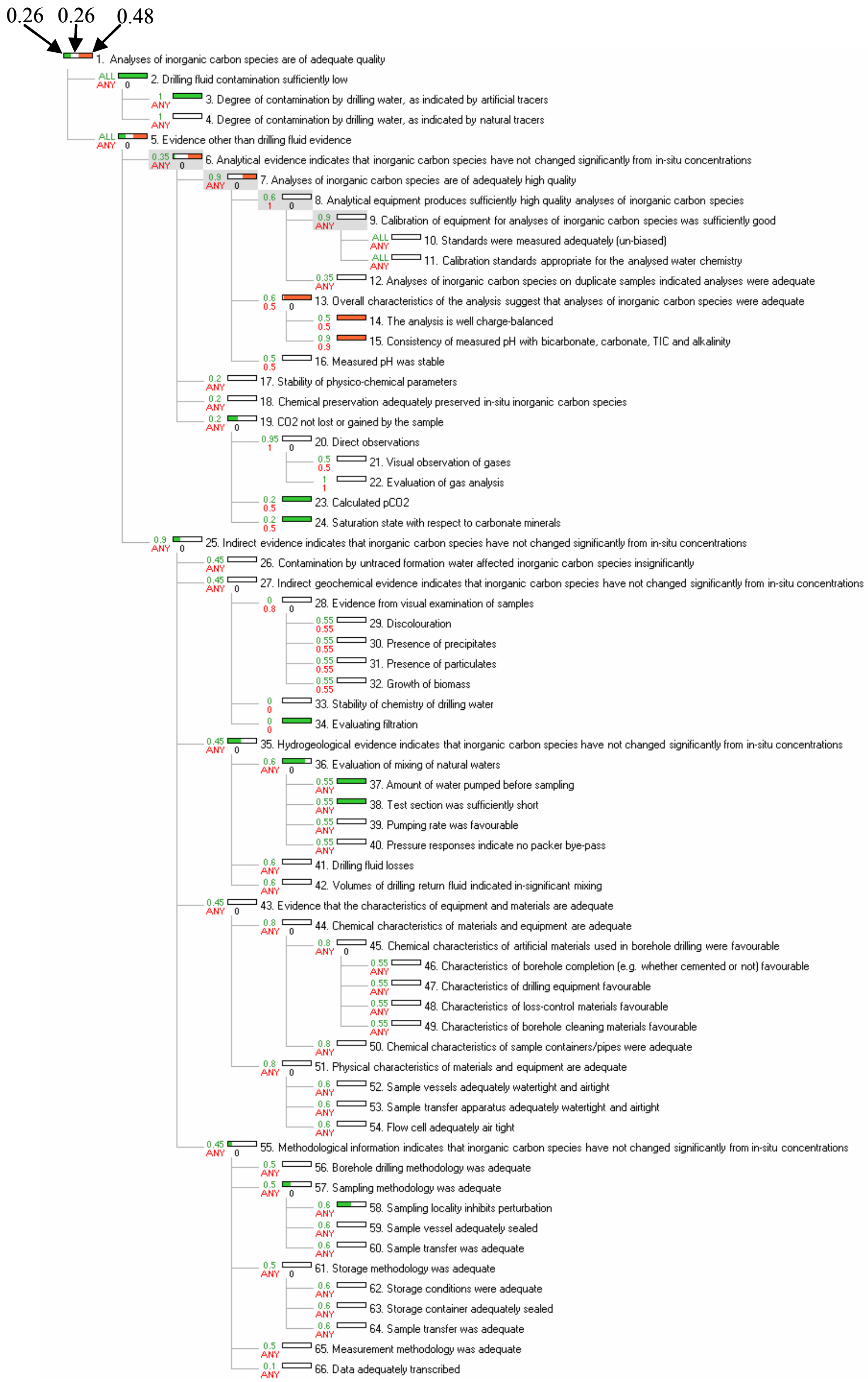


Figure 3-13 Example of a revised process model evaluating redox-sensitive trace element concentrations reported for a sample from between 15.8 m and 25.7 m depth in borehole MSB-4. In order to show the model on one page, evidence values are given only for the top level process.



1. Analyses of inorganic carbon species are of adequate quality
ALL ANY 0 2. Drilling fluid contamination sufficiently low
1 ANY 3. Degree of contamination by drilling water, as indicated by artificial tracers
1 ANY 4. Degree of contamination by drilling water, as indicated by natural tracers
ALL ANY 0 5. Evidence other than drilling fluid evidence
0.35 ANY 0 6. Analytical evidence indicates that inorganic carbon species have not changed significantly from in-situ concentrations
0.9 ANY 0 7. Analyses of inorganic carbon species are of adequately high quality
0.6 1 0 8. Analytical equipment produces sufficiently high quality analyses of inorganic carbon species
0.9 ANY 9. Calibration of equipment for analyses of inorganic carbon species was sufficiently good
ALL ANY 10. Standards were measured adequately (un-biased)
ALL ANY 11. Calibration standards appropriate for the analysed water chemistry
0.35 ANY 12. Analyses of inorganic carbon species on duplicate samples indicated analyses were adequate
0.6 0.5 0 13. Overall characteristics of the analysis suggest that analyses of inorganic carbon species were adequate
0.5 0.5 14. The analysis is well charge-balanced
0.9 0.9 15. Consistency of measured pH with bicarbonate, carbonate, TIC and alkalinity
0.5 0.5 16. Measured pH was stable
0.2 ANY 17. Stability of physico-chemical parameters
0.2 ANY 18. Chemical preservation adequately preserved in-situ inorganic carbon species
0.2 ANY 0 19. CO2 not lost or gained by the sample
0.95 1 0 20. Direct observations
0.5 0.5 21. Visual observation of gases
1 1 22. Evaluation of gas analysis
0.2 0.5 23. Calculated pCO2
0.2 0.5 24. Saturation state with respect to carbonate minerals
0.9 ANY 0 25. Indirect evidence indicates that inorganic carbon species have not changed significantly from in-situ concentrations
0.45 ANY 26. Contamination by untraced formation water affected inorganic carbon species insignificantly
0.45 ANY 0 27. Indirect geochemical evidence indicates that inorganic carbon species have not changed significantly from in-situ concentrations
0 0.8 0 28. Evidence from visual examination of samples
0.55 0.55 29. Discolouration
0.55 0.55 30. Presence of precipitates
0.55 0.55 31. Presence of particulates
0.55 0.55 32. Growth of biomass
0 0 33. Stability of chemistry of drilling water
0 0 34. Evaluating filtration
0.45 ANY 0 35. Hydrogeological evidence indicates that inorganic carbon species have not changed significantly from in-situ concentrations
0.6 ANY 0 36. Evaluation of mixing of natural waters
0.55 ANY 37. Amount of water pumped before sampling
0.55 ANY 38. Test section was sufficiently short
0.55 ANY 39. Pumping rate was favourable
0.55 ANY 40. Pressure responses indicate no packer bye-pass
0.6 ANY 41. Drilling fluid losses
0.6 ANY 42. Volumes of drilling return fluid indicated in-significant mixing
0.45 ANY 0 43. Evidence that the characteristics of equipment and materials are adequate
0.8 ANY 0 44. Chemical characteristics of materials and equipment are adequate
0.8 ANY 0 45. Chemical characteristics of artificial materials used in borehole drilling were favourable
0.55 ANY 46. Characteristics of borehole completion (e.g. whether cemented or not) favourable
0.55 ANY 47. Characteristics of drilling equipment favourable
0.55 ANY 48. Characteristics of loss-control materials favourable
0.55 ANY 49. Characteristics of borehole cleaning materials favourable
0.8 ANY 50. Chemical characteristics of sample containers/pipes were adequate
0.8 ANY 0 51. Physical characteristics of materials and equipment are adequate
0.6 ANY 52. Sample vessels adequately watertight and airtight
0.6 ANY 53. Sample transfer apparatus adequately watertight and airtight
0.6 ANY 54. Flow cell adequately air tight
0.45 ANY 0 55. Methodological information indicates that inorganic carbon species have not changed significantly from in-situ concentrations
0.5 ANY 56. Borehole drilling methodology was adequate
0.5 ANY 0 57. Sampling methodology was adequate
0.6 ANY 58. Sampling locality inhibits perturbation
0.6 ANY 59. Sample vessel adequately sealed
0.6 ANY 60. Sample transfer was adequate
0.5 ANY 0 61. Storage methodology was adequate
0.6 ANY 62. Storage conditions were adequate
0.6 ANY 63. Storage container adequately sealed
0.6 ANY 64. Sample transfer was adequate
0.5 ANY 65. Measurement methodology was adequate
0.1 ANY 66. Data adequately transcribed

Figure 3-14 Example of a revised process model showing the evaluation of inorganic carbon species reported for a sample from between 15.8 m and 25.7 m depth in borehole MSB-4. In order to show the model on one page, evidence values are given only for the top level process.

- In Figure 3-11 evidence against the adequacy of the pH measurement comes from Process 65 (‘Measurement methodology was adequate’). This process considers both the appropriateness of the measurement methodology and the degree to which it was implemented properly. In this case, the sample was analyzed in the laboratory, a method that is considered to be inappropriate for determining in-situ pH.

- In Figure 3-12 the quality of the Eh measurement is shown to be clearly inadequate. The reason for this is the fact that the measurement was made in the laboratory. Note is drawn to the fact that the measurement locality is here considered under Process 58 (‘Sampling locality inhibits perturbation’). This is in contrast to Figure 3-12, in which the measurement locality is considered under Process 65 (‘Measurement methodology was adequate’). The reason for the difference is that in the case of Eh, the measurement must be done in a flow-through cell or down-hole if useful data are to be obtained. That is, sampling locality and measurement locality amount to the same thing. However, in the case of pH (and other parameters considered with pH), measurements made in the laboratory would not be considered inadequate automatically. Instead a judgement of the quality of sampling and a judgement of the analytical methodology must be made separately.

- Comparison of Figure 3-11, Figure 3-12, Figure 3-13 and Figure 3-14 shows that drilling fluid contamination is considered to be acceptable in the cases of pH and inorganic carbon, but unacceptable in the cases of Eh and redox-sensitive trace elements.

- In Figure 3-14 the poor charge balance and inconsistency between the reported pH, TIC and alkalinity (Processes 14. and 15.) *do* contribute to the overall judgement of inorganic carbon data quality.

4 Task 3: Development of rules for choosing parameter values

4.1 Principles for choosing sufficiencies

Inevitably, an element of expert judgement is used to define the sufficiency values. Furthermore, the precise values of the sufficiencies are not important for developing a classification scheme that can be used to rank data according to its quality, as long as:

- the rationale for choosing the sufficiencies is clearly described;
- the same values are used to evaluate all available data (thus ensuring that the samples can be ranked in terms of quality).

Therefore, here, guiding principles are specified, while recognizing that the actual values will reflect expert judgement.

- As far as possible, the process model is structured so that processes considered to be equally important for evaluating quality are placed at the same level.
- Where any process failing would cause failure of the main process (e.g. evaluating whether pH data are of adequate quality), then ANY is used;
- The child processes of any parent process may represent all processes that must succeed in order for the parent to succeed. Alternatively the child processes may represent only a sub-set of these processes. The proportion of all the processes that must succeed that is represented by the actual child processes is estimated.
- Based on this estimate, the maximum possible value of 'evidence for' the parent process, if all its child processes have 'evidence for' of 1, is evaluated. For example, the main process being evaluated might be 'judging whether a groundwater sample is in-situ water'. To make this judgement, information about geochemical processes and hydrogeological processes is required. Therefore, the main process has two child processes: 'judging geochemical information'; and 'judging hydrogeological information'. If only geochemical processes are represented in the model, then the maximum 'evidence for'the parent would be 0.5.
- The 'sufficiency for' each process at a given level in the model is chosen so that if all the child processes succeeded together, the parent would succeed to the extent determined in the previous bullet point. For example, it might be judged that, if the child processes all have 'evidence for' of 1, the 'evidence for' the parent should be 0.95. The sufficiencies would be chosen to produce this result.
- If the child processes at a given level in the model are judged to be equally important for evaluating quality, then equal 'sufficiencies for' are assigned.
- If the child processes at a given level in the model are not judged to all have the same significance for quality, then 'sufficiencies for' are assigned by
    - considering the relative importance of the processes;

  - considering what overall impact is expected on the main process being evaluated.

- ▲ In most cases, the failure of a process would result in the failure of the parent process. For example, drilling fluid contamination above a certain threshold would cause the data to be rejected. For this reason, mostly the 'ANY' option is used to specify 'sufficiencies against'.

- ▲ If failure of a process or group of processes would not necessarily result in the failure of the parent, then the 'sufficiency against' is specified using the same principles as those described above in relation to 'sufficiency for'.

Except at the left-most level of the process model, the 'ALL' option is not used for sufficiencies. This is because use of the 'ALL' option results in a lack of distinction between samples with different quantities of supporting evidence. For example, the quality of pH data may depend on evidence for the quality of the analysis, evidence for lack of perturbation during borehole drilling and evidence for adequate storage conditions. If the 'ALL' option is used, then if there is no information for any one of these processes, the quality of the pH will be totally uncertain. Thus, if for one sample there is no knowledge about storage conditions and for another there is no knowledge concerning the quality of storage and the quality of analysis, then both will result in the same total uncertainty in the overall quality of pH data. From the point of view of selecting samples, for example for further analysis, it would be useful to distinguish between them. Clearly, from a probabilistic point of view, it is more likely that a sample that has been shown to be uncontaminated by reaction with borehole materials will be shown to be of adequate quality than one that has not.

4.2 Rules for assigning 'evidence' values

4.2.1 Scoping calculations

Theoretical calculations can be useful for suggesting appropriate criteria for acceptance or rejection of data, though it must be borne in mind that the results of such calculations will depend upon the water compositions used.

Drilling fluid contamination has a particularly significant effect on the quality of geochemical data. To evaluate what level of contamination would be acceptable, simple scoping calculations were carried out using the geochemical simulation codes Geochemist's Workbench (GWB, Bethke, 1996). The GWB calculations used the thermodynamic database 'thermo.tgrp', developed by JNC for the Tono Geochemistry Research Project (Iwatsuki et al., 2001).

In the GWB simulations, 1 kg of a typical drilling fluid composition (one representative of the drilling fluid used in boreholes DH-6, 7, 8, and reported in Excel file 'Table_gwchem_ver up.xls', received from JNC on 28th February 2003) was equilibrated with atmospheric O_2 (no Eh data are reported) . The simulation then 'mixed' this water with 1 kg of water with a composition based on that of groundwater from 563.75 m depth (midpoint of sampling section) in borehole DH-7 (see table in Appendix 4). The solution was charge balanced using CO_3^{2-}.

The results from these GWB simulations are illustrated in Figure 4-1 and Figure 4-2. These figures illustrate that pH is less sensitive to drilling fluid contamination than is Eh (and by inference redox-sensitive solutes). Based on the results of solubility calculations in Metcalfe et al. (2004), the solubility of most of the nuclides relevant to PA would vary relatively little over a pH range of ±0.1. Therefore, a qualifying criterion of <5% drilling fluid contamination would be reasonable. Similar mixing calculations suggest that the same criterion should also be acceptable for other determinands (major cations and anions and PA-relevant, non-redox sensitive trace constituents).

In contrast, even very small amounts of drilling fluid contamination would result in large perturbations to the Eh (Figure 4-2). These perturbations could be reflected in large changes in solubility of certain PA-relevant nuclides. Calculations presented in Metcalfe et al. (2004) showed that the solubilities of U and Tc could change by as much as 1.5 and 4 orders of magnitude respectively as a result of only 1% drilling fluid contamination.

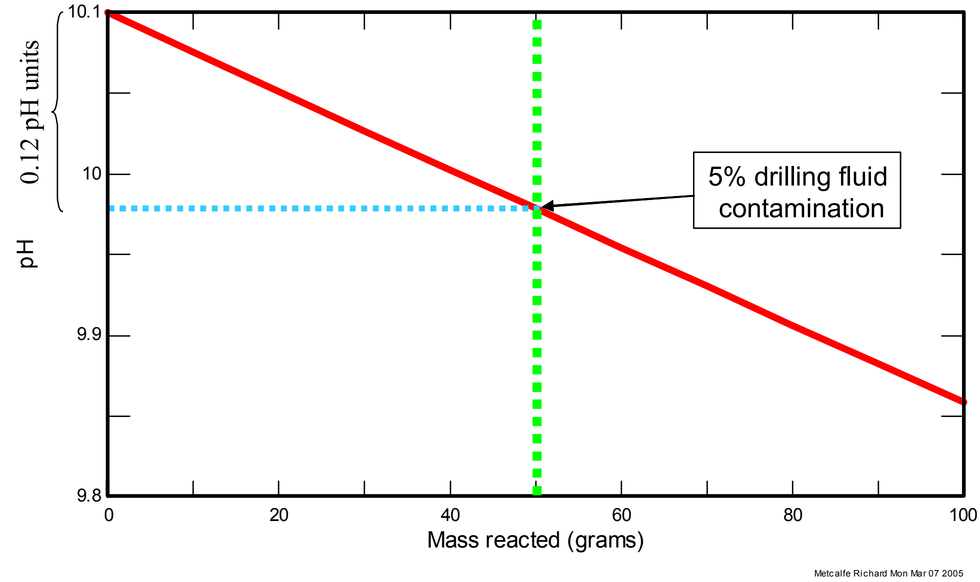


Figure 4-1 **Illustration of the effect on pH of mixing a drilling fluid with groundwater.**

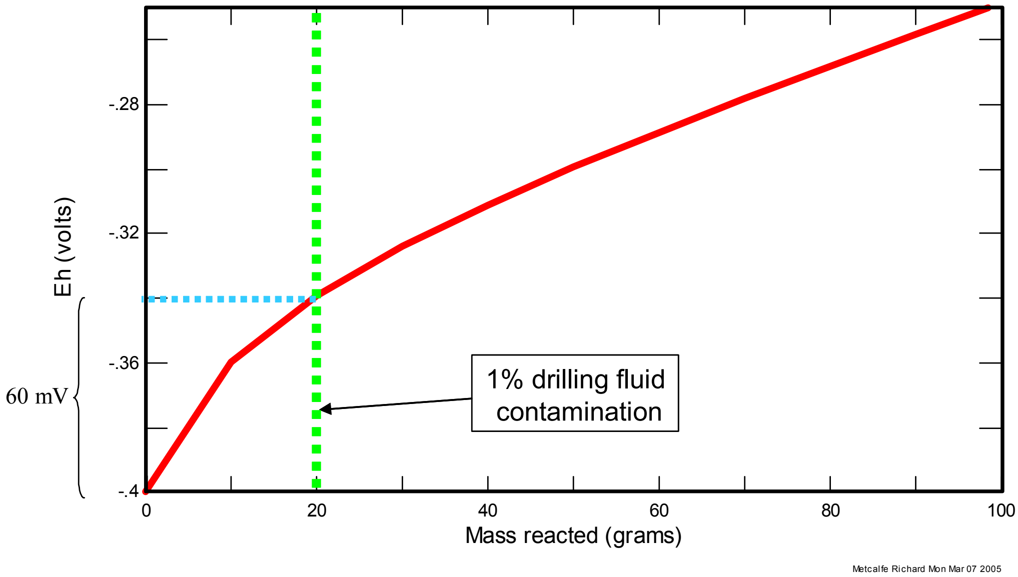


Figure 4-2 **Illustration of the effect on Eh of mixing a drilling fluid with groundwater.**

However, to reject Eh data simply because the drilling fluid contamination is greater than 1% would be overly stringent and result in useful information being lost. Even though 1% drilling fluid contamination might perturb the Eh by several tens of mV, as in Figure 4-2, this range is much smaller than the range of Eh values observed in natural groundwater systems (typically several 100 mV). Furthermore, the uncertainty could caused by the contamination could be taken into account by probabilitistic PA techniques.

For these reasons, it is suggested that a qualifying criterion of <1% drilling fluid contamination would be reasonable for an initial selection of Eh values from a dataset. However, further selection of samples based on a more stringent criterion might be appropriate at a later stage, depending upon the purpose of using the data.

In the cases of the redox-sensitive trace constituents (Fe^{2+}, Fe^{3+}, HS^- etc) a more stringent criterion is justified since their concentrations will be perturbed by the presence of even trace amounts of oxygen. It is suggested that in this case, drilling fluid contamination should be below 0.1%.

Simulations were also carried out using PHREEQC version 2.8 (Parkhurst and Appelo, 1999) to evaluate what degree of consistency would be appropriate for alkalinity, TIC and pH. In this case the thermodynamic database llnl.dat, which is distributed with the PHREEQC package was used. It was not possible to use JNC’s PHREEQC-formatted database since this does not support calculations of alkalinity.

The composition of the sample from between 437.6 m and 462.1 m depth in borehole DH-15 was used as a basis for the calculations. Initially, the simulation was carried out using only TIC to constrain the dissolved carbon species. The code calculated an alkalinity based on this composition. Then, this alkalinity value was added back into the original analysis (which therefore contained both a TIC concentration and an alkalinity value).

When PHREEQC takes both alkalinity and TIC as input, it adjusts pH to achieve a match between the dissolved carbon species and the alkalinity. Initially, the three values were self-consistent, by definition, and so a further simulation would not change the pH. However, the alkalinity value was progressively deviated from the initial consistent value and the effect on the calculated pH was determined. The results are shown in Figure 4-3.

This figure shows that for this sample, a deviation of alkalinity of about 3% from the initial (consistent) value would cause a change in pH of about 0.1 units. For the reasons discussed above in connection with drilling fluid contamination, a deviation of this small amount would probably be acceptable. Therefore a consistency between measured and calculated alkalinity of within 3% is taken as an acceptability criterion.

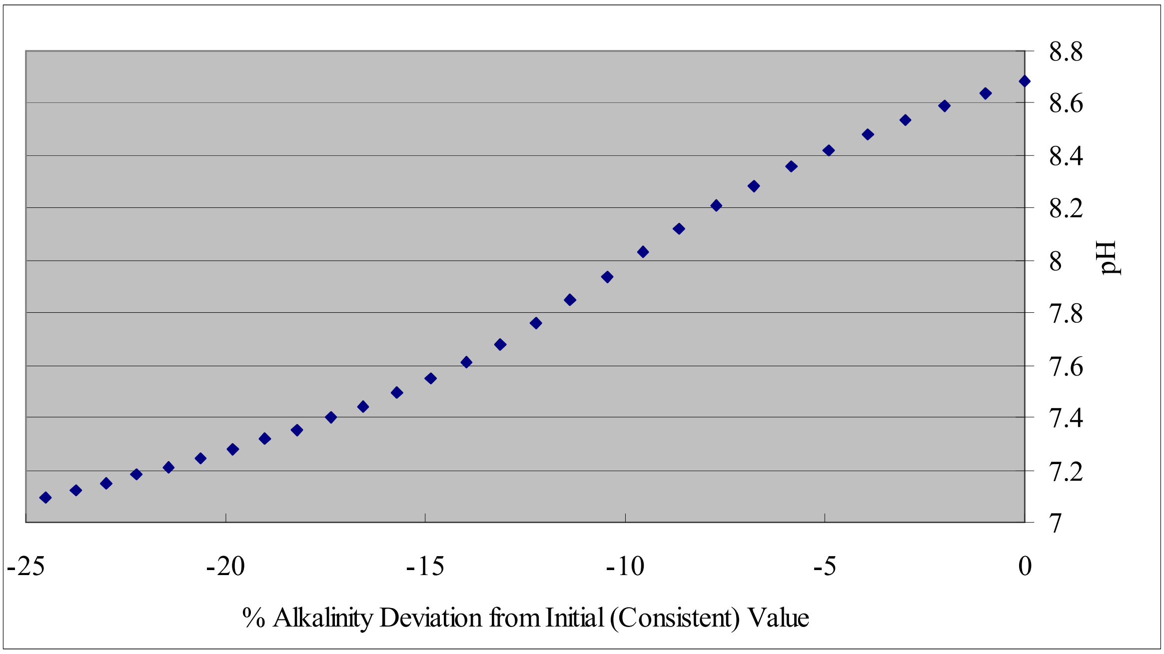


Figure 4-3 Results from a PHREEQC simulation investigating the significance of inconsistencies between alkalinity, pH and TIC. The pH is plotted against the percentage deviation in the alkalinity from the initial value in the illustration below.

4.2.2 Definition of rules for assigning evidence values

The following general principles are adopted.

- Where a particular process is clearly related to the overall process being evaluated (e.g. assessment of pH data) and related to a numerical criterion (e.g. 5% drilling fluid contamination), then if the criterion is met an 'evidence for' value of 1 is assigned. Failure to meet the criterion is represented by 'evidence against' of 1.

- If the process is irrelevant for the particular sample being considered (e.g. Process 12. 'Measurement of pH on duplicate standards indicated pH measurements were adequate', when the pH was measured in a flow-through cell), then an 'evidence for' value of 1 is assigned.

- Where expert judgement is required to ascertain whether or not a criterion is met, it would be appropriate to construct sub-process models to evaluate the 'evidence for' and 'evidence against'. However, such an approach might be impractical to implement for large datsets. Therefore a pragmatic solution is suggested whereby:

- criterion for success is probably met, then 'evidence for' is 1;
- crierion for success is probably not met, then the 'evidence against' is 1;
- criterion for success is possibly met, then 'evidence for' is 0.5;
- criterion for success is possibly not met, then 'evidence against' is 0.5
- where appropriate, textual justifications for the assignment of values are entered into the process models

More specific rules for assigning evidence values are given in Table 4-1.

The rules applied to processes in the other process models are very similar. Differences between these process models and the model used to evaluate pH are listed in Table 4-2, Table 4-3, and Table 4-4.

A particular difficulty occurs in the case of evaluating hydrogeological information that may indicate the extent to which a sample is representative of the undisturbed (pre-sampling) conditions. In the present work, the only such information used was:

- ▲ the length of the test section;
- ▲ the amount of the water pumped.

A rigorous evaluation of the significance of these quantities needs to be made on a test-be-test basis and take into account information about the permeability structure of the rock mass (e.g. fracture distributions, frequencies and hydraulic characteristics) and the groundwater potential field. It is also necessary to consider the spatial variations in groundwater chemistry around the sampled interval. The greater the variability in chemistry, the shorter will be the section that can be tested, and the smaller will be the quantity of water that can pumped, without perturbing in-situ chemical conditions by mixing. Such detailed evaluations were beyond the scope of this work. However, to illustrate the general importance of evaluating the effects of groundwater mixing on the 'representativeness' of a groundwater analysis, a pragmatic approach was adopted whereby:

- ▲ If the amount of water pumped was < 10,000 l, Process 37. ('Amount of water pumped before sampling') was given an 'evidence for' value of 1.0.
- ▲ If the amount of water pumped was > 10,000 l and < 50,000 l, Process 37. was given an 'evidence against' value of 0.5.
- ▲ If the amount of water pumped was > 50,000 l, Process 37. was given an 'evidence against' value of 1.0.

- ▲ If the test section was < 10 m in length, Process 38. ('Test section was sufficiently short' was given an 'evidence for') value of 1.0.
- ▲ If the test section was > 10 m and < 25 m in length, Process 38. was given an 'evidence against' value of 0.5.
- ▲ If the test section was > 25 m in length, Process 38. was given an 'evidence against' value of 1.0.

It is noted that a disadvantage of this scheme is that there is no gradation in evidence values and 'evidence for' suddenly 'flips' to become evidence again at fixed values.

The criteria for success or failure of Process 16. ('Measured pH (or Eh) was stable') and 17. ('Stability of physico-chemical parameters') are rigorously defined in Table 4-1, Table 4-2, Table 4-3 and Table 4-4. However, sufficient information to judge these processes rigorously was available only for samples from boreholes KNA-6 and DH-15. Stability information for many other samples was available only in the form of rates of change of pH, Eh and EC, averaged over intervals of 5 hours (Table 5-1, Table A4.2). In the absence of information concerning long-term trends, these rates do not enable the stability of these parameters to be evaluated confidently. Nevertheless, these rates do provide useful information. Therefore, the following criteria were adopted:

- ▲ 'Evidence for' of 0.5 was assigned to Processes 16., considering pH or Eh as appropriate, if:
  - pH changed by < 0.001 pH units per hour;
  - Eh changed by < 0.5 mV per hour;
  - EC changed by < 0.5 mS m^{-1} per hour.
- ▲ 'Evidence against' of 0.5 was assigned to Processes 16., considering pH or Eh as appropriate, if:
  - pH changed by > 0.001 pH units per hour;
  - Eh changed by > 0.5 mV per hour;
  - EC changed by > 0.5 mS m^{-1} per hour.

The criteria for pH and Eh are values of 1% of the acceptable variation in these parameters, as discussed in Section 4.2.1 . The criteria for EC is approximately 1% of the range of deviation seen in borehole DH-15.

Process 17. ('Stability of physico-chemical parameters') refers to both EC and temperature. There are no data reported for the stability of the latter and therefore the judgement must be based only on stability information for EC. The values are assigned as follows:

- ‘Evidence for’ of 0.25 was assigned to Processes 17 if EC changed by < 0.5 mS m^{-1} per hour.

- ‘Evidence against’ of 0.25 was assigned to Processes 17 if EC changed by > 0.5 mS m^{-1} per hour.

It is emphasised once again that these criteria are pragmatic criteria, chosen for the purposes of illustrating the data quality classification method.

Table 4-1 Rules for assigning 'evidence for' and 'evidence against' each process corresponding to a data quality indicator in the process model for evaluating pH. (Figure 3-11). Only those processes at the right, into which the user would add evidence values, are considered.

Process No	Quality indicator	Rule for assigning 'evidence for' and 'evidence against'
3.	Degree of contamination by drilling water, as indicated by artificial tracers (e.g. fluorescent dye insignificant)	If the contamination is <5%, then the evidence for is 1; otherwise evidence against is 1.
4.	Degree of contamination by drilling water, as indicated by natural tracers	If there is no detectable degree of contamination by drilling water, as indicated by natural tracers (e.g. tritium) *and* there are known to be suitable tracers in the drilling fluid, then evidence for is 1. If there is detectable contamination by drilling water, as indicated by natural tracers (e.g. tritium) then evidence against is 1.
10.	Standards were measured adequately (un-biased)	If analytical standards were measured and results shown to be within accepted values, then 'evidence for' is 1, otherwise 'evidence against' is 1.
11.	Calibration standards appropriate for the analysed water chemistry	If the calibration standards were appropriate for the analysed water chemistry, then evidence for is 1, otherwise evidence against is 1.
12.	Measurement of pH on duplicate standards indicated pH measurements were adequate	If duplicate analyses on the same sample gave results within analytical precision, then evidence for is 1, otherwise evidence against is 1.
14.	The analysis is well charge-balanced	If the charge is within 5% of balanced then evidence for is 1, otherwise evidence against is 1.
15.	Consistency of measured pH with bicarbonate, carbonate, TIC and alkalinity	If the calculated and measured alkalinity and pH are consistent to within 3% (for any 1 parameter calculated using the other two), then evidence for is 1, otherwise evidence against is 1.
16.	Measured pH was stable	If the pH did not show any systematic drift during measurement and any fluctuations were comparable with the analytical error, then the evidence for is 1, otherwise the evidence against is 1.
17.	Stability of physico-chemical parameters	If at the time of measurement (or sample collection, if the pH was measured in the laboratory), the physico-chemical parameters (temperature, EC) were not varying with any trend and showed fluctuations comparable with the analytical error, then evidence for is 1, otherwise, evidence against is 1.
18.	Chemical preservation adequately preserved in-situ pH	If the pH was analysed in the laboratory and any chemical preservation did not perturb pH, then evidence for is 1. Alternatively, if analysed in a flow-through cell so that preservation was not performed, then evidence for is 1. Alternatively, if any preservatives were added that would perturb the pH, then evidence against is 1.
21.	Visual observation of gases	If no gas is evolved then evidence for is 1. If gas is evolved then evidence against is 1.

Table 4-1 continued.

Process No	Quality indicator	Rule for assigning 'evidence for' and 'evidence against'
22.	Evaluation of gas analysis	If gas is evolved and shown to contain no CO_2, then evidence for is 1. If gas is evolved and shown to contain CO_2, then evidence against is 1.
23.	Calculated pCO_2	If substantially different from the atmospheric value ($\log pCO_2 = -3.15$) then evidence for is 1. If the same as the atmospheric value, then evidence against is 1.
24.	Saturation state with respect to carbonate minerals	If saturated with respect to calcite (saturation index within +/- 0.2) then evidence for is 1, otherwise evidence against is 1.
26.	Contamination by untraced formation water affected pH insignificantly	If contamination by untraced formation water (based on analysis of pumped water volumes and time-dependent changes in chemistry) is definitely insignificant (does not affect pH by more than 0.1 pH units), then evidence for is 1. If contamination by untraced formation water is possibly significant, then evidence against is 0.5. If contamintaion by untraced formation water is probably significant, then evidence against is 1.
29.	Discolouration	If the sample is not discoloured, then evidence for is 1, othewise evidence against is 1.
30.	Presence of precipitates	If precipitates are not present in the sample, then evidence for is 1, otherwise evidence against is 1.
31.	Presence of particulates	If particulates are absent, then evidence for is 1, otherwise evidence against is 1.
32.	Growth of biomass	If no biomass can be observed in the sample, then evidence for is 1, otherwise evidence against is 1.
33.	Stability of chemistry of drilling water	If the chemistry of the drilling water was sufficiently stable that contamination is likely to have been simply two-component mixing, then evidence for is 1. If the chemistry of the drilling water was possibly not sufficiently stable, to result in two-component mixing, then evidence against is 0.5. If the chemistry of the drilling water was probably not sufficiently stable, to result in two-component mixing, then evidence against is 0.5.
34.	Evaluating filtration	If filtering of the sample probably did not perturb pH by more than 0.1 pH units, then evidence for is 1, If filtering was not required, because the pH was measured in a flow-through cell, then evidence for is 1. If filtering possibly caused a perturbation of the pH of > 0.1 pH units, then evidence against is 0.5. If filtering definitely caused a perturbation of the pH of > 0.1 pH units, then evidence against is 1.

Table 4-1 continued.

Process No	Quality indicator	Rule for assigning 'evidence for' and 'evidence against'
37.	Amount of water pumped before sampling	If it is judged that the amount of water pumped before sampling is insufficient to cause mixing between chemically different groundwater samples, then evidence for is 1. If it is judged that the amount of water pumped before sampling is sufficient to make mixing between chemically different groundwater samples possible, then evidence against is 0.5. If it is judged that the amount of water pumped before sampling is sufficient to make mixing between chemically different groundwater samples probable, then the evidence against is 1.
38.	Test section was sufficiently short	If it is judged that the test section is insufficiently long to allow mixing between chemically different groundwater samples, then evidence for is 1. If it is judged that the test section is sufficiently long to make mixing between chemically different groundwater samples possible, then evidence against is 0.5. If it is judged that the test section is sufficiently long to make mixing between chemically different groundwater samples probable, then the evidence against is 1.
39.	Pumping rate was favourable	If it is judged that the pumping rate was sufficiently low to prevent inducing mixing between chemically different groundwater samples (e.g. by cross-formational flow), then evidence for is 1. If it is judged that the pumping rate was sufficiently fast to possibly induce mixing between chemically different groundwater samples (e.g. by cross-formational flow), then evidence against is 0.5. If it is judged that the pumping rate was sufficiently fast to probably induce mixing between chemically different groundwater samples, then the evidence against is 1.
40.	Pressure responses indicate no packer bye-pass	If pressure responses indicated no packer bye-pass, then evidence for is 1, otherwise evidence against is 1.
41.	Drilling fluid losses	If drilling fluid losses were not sufficiently large to have caused mixing between chemically different natural groundwater bodies, then evidence for is 1. If drilling fluid losses were possibly sufficiently large to have caused mixing between chemically different natural groundwater bodies, then evidence against is 0.5. If drilling fluid losses were probably sufficiently large to have caused mixing between chemically different natural groundwater bodies, then evidence against is 1.

Table 4-1 continued.

Process No	Quality indicator	Rule for assigning 'evidence for' and 'evidence against'
42.	Volumes of drilling return fluid indicated in-significant mixing	If the volumes of drilling return fluid do not indicate significant inflow of natural groundwater to the borehole and with it the implication of mixing between chemically different natural groundwater bodies, then evidence for is 1. If the volumes of drilling return fluid possibly indicate significant inflow of natural groundwater to the borehole and with it the implication of mixing between chemically different natural groundwater bodies, then evidence against is 0.5. If the volumes of drilling return fluid probably indicate significant inflow of natural groundwater to the borehole and with it the implication of mixing between chemically different natural groundwater bodies, then evidence against is 0.5.
46.	Characteristics of borehole completion (e.g. whether cemented or not) favourable	If cement would not react so as to perturb pH, then evidence for is 1. If cement was not used, then evidence for is 1. If cement could possibly have reacted so as to perturb pH, then evidence against is 0.5, If cement probably reacted so as to perturb pH, then evidence against is 1.
47.	Characteristics of drilling equipment favourable	If drilling equipment would not react so as to perturb pH, then evidence for is 1. If drilling equipment could possibly have reacted so as to perturb pH, then evidence against is 0.5, If drilling equipment probably reacted so as to perturb pH, then evidence against is 1.
48.	Characteristics of loss-control materials favourable	If loss control materials would not react so as to perturb pH, then evidence for is 1. If loss control materials were not used, then evidence for is 1. If loss control materials could possibly have reacted so as to perturb pH, then evidence against is 0.5, If loss control materials probably reacted so as to perturb pH, then evidence against is 1.
50.	Chemical characteristics of sample containers/ pipes were adequate	If the sample containers and pipes used were not reactive, then evidence for is 1, otherwise evidence against is 1.
52.	Sample vessels adequately watertight and airtight	If sample vessels were watertight and airtight, evidence for is 1, otherwise evidence against is 1.
53.	Sample transfer apparatus adequately watertight and airtight	If the sample transfer was adequately watertight and airtight, then evidence for is 1, otherwise evidence against is 1.
54.	Flow cell adequately air tight	If the flow-through cell was adequately air-tight, evidence for is 1. If a flow-through cell was not used, then evidence for is 1. If the flow-through cell was not adequately air-tight, then evidence against is 1.

Table 4-1 continued.

Process No	Quality indicator	Rule for assigning 'evidence for' and 'evidence against'
56.	Borehole drilling methodology was adequate	If the borehole drilling methodology (including completion and cleaning etc) probably did not significantly perturb either the chemistry or spatial distribution of groundwater, then evidence for is 1. If the borehole drilling methodology (including completion and cleaning etc) possibly significantly perturbed either the chemistry or spatial distribution of groundwater, then evidence against is 0.5. If the borehole drilling methodology (including completion and cleaning etc) probably significantly perturbed either the chemistry or spatial distribution of groundwater, then evidence against is 1.
58.	Sampling locality inhibits perturbation	If the sample was collected downhole, then evidence for is 1. If the measurement locality (for pH) was downhole, then evidence for is 1. If the measurement locality (for pH or Eh) was at the surface and the values showed long-term stability, then evidence for is 1. If the sample was collected at the surface in a way that inhibited perturbation, then evidence for is 0.5. If the measurement locality was a surface flow-through cell (for pH), but there is no evidence for long-term stability, then evidence for is 0.5. If there is any evidence that perturbation was likely at the sampling locality, then evidence against is 1.
59.	Sample vessel adequately sealed	If the sample vessel was sealed so as to prevent ingress of air or evaporation, then evidence for is 1, otherswise evidence against is 1.
60.	Sample transfer was adequate	If sample transfer did not allow leakage, then evidence for is 1, otherwise evidence against is 1.
62.	Storage conditions were adequate	If the storage conditions adequately prevented perturbations to the sample's chemistry, then evidence for is 1. If the storage conditions possibly allowed perturbations to the sample's chemistry, then evidence against is 0.5. If the storage conditions probably allowed perturbations to the sample's chemistry, then evidence against is 1.
63.	Storage container adequately sealed	If the storage container adequately prevented leakage, then evidence for is 1. If the storage conditions possibly allowed leakage, then evidence against is 0.5. If the storage conditions probably allowed leakage, then evidence against is 1.
64.	Sample transfer was adequate	If sample transfer adequately prevented leakage, then evidence for is 1. If sample transfer possibly allowed leakage, then evidence against is 0.5. If sample transfer probably allowed leakage, then evidence against is 1.

Table 4-1 continued.

Process No	Quality indicator	Rule for assigning 'evidence for' and 'evidence against'
65.	Measurement methodology was adequate	If the measurement methodology was appropriate and properly implemented, then evidence for is 1. If the measurement methodology was inappropriate and/or possibly not properly implemented, then evidence against is 0.5. If the measurement methodology was probably inappropriate and/or not properly implemented, then evidence against is 1.
66.	Data adequately transcribed	If the data have been checked for transcription errors, then evidence for is 1, otherwise no evidence is entered.

Table 4-2 Summary of the differences between the ESL process model for evaluating Eh (Figure 3-12) and the ESL process model for evaluating pH (Figure 3-11). Differences in process titles are highlighted in red.

Item	Eh process model (e.g. Figure 3-12)
Process titles	Process 6 'Analytical evidence indicates that pH has not changed significantly from in-situ value' changed to 'Analytical evidence indicates that Eh has not changed significantly from in-situ value' Process 7 'pH measurement is of adequately high quality' changed to 'Eh measurement is of adequately high quality' Process 8 'Analytical equipment produces sufficiently high quality pH data' changed to 'Analytical equipment produces sufficiently high quality Eh data' Process 9 'pH calibration was sufficiently good' changed to 'Eh calibration was sufficiently good' Process 12 'Measurement of pH on duplicate samples indicated pH measurements were adequate' changed to 'Measurement of Eh on duplicate samples indicated Eh measurements were adequate' Process 13. 'Overall characteristics of the analysis suggest that pH measurements were adequate' changed to 'Overall characteristics of the analysis suggest that Eh measurements were adequate' Process 18. 'Chemical preservation adequately preserved in-situ pH' changed to 'Chemical preservation adequately preserved in-situ Eh' Process 25. 'Indirect evidence indicates that pH has not changed significantly from in-situ value' changed to 'Indirect evidence indicates that Eh has not changed significantly from in-situ value' Process 26. 'Contamination by untraced formation water affected pH insignificantly' changed to 'Contamination by untraced formation water affected Eh insignificantly' Process 27. 'Indirect geochemical evidence indicates that pH has not changed significantly from in-situ value' changed to 'Indirect geochemical evidence indicates that Eh has not changed significantly from in-situ value' Process 35. 'Hydrogeological evidence indicates that pH has not changed significantly from in-situ value' changed to 'Hydrogeological evidence indicates that Eh has not changed significantly from in-situ value' Process 55. 'Methodological information indicates that pH has not changed significantly from in-situ value' changed to 'Methodological information indicates that Eh has not changed significantly from in-situ value'

Table 4-2 continued.

Item	Eh process model (e.g. Figure 3-12)
Process model structure	**Processes added** Child Process 1a ('Drilling fluid contamination sufficiently low') added to Process 1 ('Eh measurement is of adequate quality') Child Process 58a ('Measurement made in well-head flow cell') added to Process 58. ('Sampling locality inhibits perturbation') Child Process 58b ('Measurement madedownhole') added to Process 58. ('Sampling locality inhibits perturbation') **Processes moved** Process 2 ('Drilling fluid contamination sufficiently low') was a child of Process 1. ('pH measurement is of adequate quality'), but becomes a child process of Process 1a ('Drilling fluid contamination sufficiently low') Process 58. ('Sampling locality inhibits perturbation') was a child of Process 57. ('Sampling methodology was adequate'), but becomes a child of Process 1a
Sufficiencies	Process 58. ('Sampling locality inhibits perturbation'): For changed from 0.6 to ANY Process 58a. ('Measurement made in well-head flow cell'): For = 1 if long-term monitoring and shown to be stable; 0.5 if no long-term monitoring; Against = ALL Process 58b. ('Measurement made downhole'): For = 1; Against = ALL Process 9. ('Eh calibration was sufficiently good'): For changed from 0.9 to 1 Process 12. ('Measurement of pH on duplicate standards indicated Eh measurements were adequate'): For changed from 0.35 to 0 Process 17. ('Stability of physico-chemical parameters'): For changed from 0 to 0.25; Against changed from 0 to ANY Process 18. ('Chemical preservation adequately preserved in-situ Eh'): For changed from 0.2 to 0 Process 19. ('CO_2 not lost or gained by the sample'): For changed from 0.2 to 0.25 Process 57. ('Sampling methodology was adequate'): For changed from 0.5 to 0 Process 61. ('Storage methodology was adequate'): For changed from 0.5 to 0; Against changed from ANY to 0
Changes to criteria	Process 3. ('Degree of contamination by drilling water, as indicated by artificial tracers') Criterion for success changed from <5% drilling fluid contamination to <1% drilling fluid contamination.

Table 4-3 Summary of the differences between the ESL process model for evaluating redox-sensitive trace elements (Figure 3-13) and the ESL process model for evaluating pH (Figure 3-11). Differences in process titles are highlighted in red.

Item	Redox-sensitive elements process model (e.g. Figure 3-13)
Process titles	Process 6 'Analytical evidence indicates that pH has not changed significantly from in-situ value' changed to 'Analytical evidence indicates that redox-sensitive solutes have not changed significantly from in-situ value' Process 7 'pH measurement is of adequately high quality' changed to 'Analyses of redox-sensitive solutes are is of adequately high quality' Process 8 'Analytical equipment produces sufficiently high quality pH data' changed to 'Analytical equipment produces sufficiently high quality data for redox-sensitive solutes' Process 9 'pH calibration was sufficiently good' changed to 'Calibration for redox-sensitive solutes was sufficiently good' Process 12 'Measurement of pH on duplicate samples indicated pH measurements were adequate' changed to 'Analyses of redox-sensitive solutes on duplicate samples were adequate' Process 13. 'Overall characteristics of the analysis suggest that pH measurements were adequate' changed to 'Overall characteristics of the analysis suggest that analyses of redox-sensitive solutes were adequate' Process 18. 'Chemical preservation adequately preserved in-situ pH' changed to 'Chemical preservation adequately preserved in-situ redox-sensitive solutes' Process 25. 'Indirect evidence indicates that pH has not changed significantly from in-situ value' changed to 'Indirect evidence indicates that redox-sensitive solutes have not changed significantly from in-situ value' Process 26. 'Contamination by untraced formation water affected pH insignificantly' changed to 'Contamination by untraced formation water affected redox-sensitive solutes insignificantly' Process 27. 'Indirect geochemical evidence indicates that pH has not changed significantly from in-situ value' changed to 'Indirect geochemical evidence indicates that redox-sensitive solutes have not changed significantly from in-situ value' Process 35. 'Hydrogeological evidence indicates that pH has not changed significantly from in-situ value' changed to 'Hydrogeological evidence indicates that redox-sensitive solutes have not changed significantly from in-situ value' Process 55. 'Methodological information indicates that pH has not changed significantly from in-situ value' changed to 'Methodological information indicates that redox-sensitive solutes have not changed significantly from in-situ value'
Process model structure	**Processes added** None **Processes moved** None

Table 4-3 continued.

Item	Redox-sensitive elements process model (e.g. Figure 3-13)
Sufficiencies	Process 16. ('Measured pH was stable'): For changed from 0.5 to 0 Process 17. ('Stability of physico-chemical parameters'): For changed from 0 to 0.2; Against changed from 0 to ANY
Changes to criteria	Process 3. ('Degree of contamination by drilling water, as indicated by artificial tracers') Criterion for success changed from <5% drilling fluid contamination to <0.1% drilling fluid contamination.

Table 4-4 Summary of the differences between the ESL process model for evaluating inorganic carbon species (Figure 3-14) and the ESL process model for evaluating pH (Figure 3-11). Differences in process titles are highlighted in red.

Item	Analysis of inorganic carbon species process model (e.g. Figure 3-14)
Process titles	Process 6 'Analytical evidence indicates that pH has not changed significantly from in-situ value' changed to 'Analytical evidence indicates that inorganic carbon species have not changed significantly from in-situ value' Process 7 'pH measurement is of adequately high quality' changed to 'Analyses of inorganic carbon species are of adequately high quality' Process 8 'Analytical equipment produces sufficiently high quality pH data' changed to 'Analytical equipment produces sufficiently high quality analyses of inorganic carbon species' Process 9 'pH calibration was sufficiently good' changed to 'Calibration of equipment for analyses of inorganic carbon species was sufficiently good' Process 12 'Measurement of pH on duplicate samples indicated pH measurements were adequate' changed to 'Analyses of inorganic carbon species on duplicate samples were adequate' Process 13. 'Overall characteristics of the analysis suggest that pH measurements were adequate' changed to 'Overall characteristics of the analysis suggest that analyses of inorganic carbon species were adequate' Process 18. 'Chemical preservation adequately preserved in-situ pH' changed to 'Chemical preservation adequately preserved in-situ inorganic carbon species' Process 25. 'Indirect evidence indicates that pH has not changed significantly from in-situ value' changed to 'Indirect evidence indicates that inorganic carbon species have not changed significantly from in-situ value' Process 26. 'Contamination by untraced formation water affected pH insignificantly' changed to 'Contamination by untraced formation water affected inorganic carbon species insignificantly' Process 27. 'Indirect geochemical evidence indicates that pH has not changed significantly from in-situ value' changed to 'Indirect geochemical evidence indicates that inorganic carbon species have not changed significantly from in-situ concentrations' Process 35. 'Hydrogeological evidence indicates that pH has not changed significantly from in-situ value' changed to 'Hydrogeological evidence indicates that inorganic carbon species have not changed significantly from in-situ value' Process 55. 'Methodological information indicates that pH has not changed significantly from in-situ value' changed to 'Methodological information indicates that inorganic carbon species have not changed significantly from in-situ value'

Table 4-4 continued.

Item	Analysis of inorganic carbon species process model (e.g. Figure 3-14)
Process model structure	**<u>Processes added</u>** None **<u>Processes moved</u>** None
Sufficiencies	Process 7. ('Analyses of inorganic carbon species are of adequately high quality'): Against changed from 1 to ANY Process 8. ('Analytical equipment produces sufficiently high quality analyses of inorganic carbon species'): Against changed from ANY to 1 Process 13. ('Overall characteristics of the analysis suggest that analyses of inorganic carbon species were adequate'): For changed from 0 to 0.6; Against changed from ANY to 0.5 Process 14. ('The analysis is well charge-balanced'): For changed from 0.8 to 0.5; Against changed from 0 to 0.5 Process 15. ('Consistency of measured pH with bicarbonate, carbonate, TIC and alkalinity'): For changed from 0.8 to 0.9; Against changed from 0 to 0.9 Process 16. ('Measured pH was stable'): For changed from 0.8 to 0.5; Against changed from ANY to 0.5 Process 17. ('Stability of physico-chemical parameters'): For changed from 0 to 0.2; Against changed from 0 to ANY Process 18. ('Chemical preservation adequately preserved in-situ inorganic carbon species'): Against change from 1 to ANY Process 19. ('CO_2 not lost or gained by the sample'): Against change from 1 to ANY Process 57. ('Sampling methodology was adequate'): For changed from 0.5 to 0 Process 61. ('Storage methodology was adequate'): For changed from 0.5 to 0; Against changed from ANY to 0
Changes to criteria	None

5 Task 4. Classification of existing data

The data quality classification method has been applied to:

- all data in and immediately surrounding the MIU site, from boreholes DH-2, MIZ-1, DH-15, MSB-2 and MSB-4.
- a selection of data from other boreholes, KNA-6, DH-7, DH-12 and MIU-4.

The data considered, associated quality information and resulting quality classification are given in Appendix 4. It is stressed that the classification is made based upon the quality information available to the author. It is likely that many other relevant data exist, for example documentary records of sampling and analytical techniques. An important feature of the TESLA program is that it allows the process models to be up-dated rapidly as more quality information become available. Consequently, the quality evaluation presented here could be revised readily.

In this section, the classification scheme is applied to a sub-set of the data (Table 5-1). The results are summarized in Table 5-2 and in Figure 3-11 to Figure 3-14 and in Figure 5-1 to Figure 5-12.

In Table 5-2 the quality of each determinand is indicated by a combination of the ratio ‘evidence for the quality being adequate’/’evidence against the quality being adequate’, and the residual uncertainty. In some cases, the latter is a negative number. Such a situation reflects conflict in the evidence for and against (i.e. the values sum to >1). Conflicts of this type can be seen in Figure 5-5, Figure 5-6, Figure 5-8 and are perfectly permissible in the ESL method where they highlight genuine conflicts of information. In the case of the sample from between 171.8 and 280.2 m in borehole DH-12 (Figure 5-5), the conflict occurs because the geochemical evidence generally indicates adequate pH quality, but the hydrogeological evidence (length of sampling section and amount of water pumped) indicates that the pH is not representative of the sampling locality. Thus, in this case, the conflict highlights that different kinds of information indicate different things about the data quality.

The greatest quantity of quality information were available for borehole KNA-6 (Figure 5-1). In this case, additional quality information, besides that in Table 5-1, was taken from Ota and Hanamuro (1996).

The KNA-6 data were obtained from water sampled during long-term (c. 100 days) monitoring. Consequently, the quality indicators also generally high quality data, with the result that the overall judgement indicates high quality with low uncertainty.

Table 5-1 Quality information for a sub-set of samples used to illustrate the quality classification system.

Index	Location	Depth			During sampling				During analysis			
		Min	Middle	Max	Smell	Colour change	Gas bubbles	Precipitation	Smell	Colour change	Gas bubbles	Precipitation
Units		mbgl	mbgl	mbgl								
AKEYO F.												
168	MSB-4	15.8	20.75	25.7								
LOWER TOKI LIGNITE-BEARING FORMATION/TOKI GRANITE												
2	KNA-6 unconf.	-										
LOWER TOKI LIGNITE-BEARING FORMATION												
165	MSB-2	132.0	142.99	154.0	A little	No	Yes	No	A little	No	No	No
TOKI GRANITE												
173	DH-2	305.6	306.55	307.6								
108	DH-7	560.5	563.75	567.0								
151	DH-12	171.8	225.99	280.2								
162	MIU-4	505.8	533.09	560.4	No	No	No	No	No	No	No	No
166	MSB-2	171.5	173.49	175.5	A little	No	Yes	No	A little	No	No	No
	MIZ-1	215.0	220.34	225.7	Hydrogen sulfide	No	Yes	No	Hydrogen sulfide	No	No	No
	DH-15	437.60	449.85	462.1	Weak	Light pink	Yes	No	Weak	Light pink	Yes	No

Table 5-1 continued.

Index	Location	Depth			Drilling fluid tracers			Drilling fluid contamination	Charge balance	Sample container	Stability of pH	Stability of EC	Stability of Eh	Distance between packers
		Min	**Middle**	**Max**	**Uranine Tracer**	**Amino-G acid**	**Eosin**	**%**	**%**		**/hour**	**mS/m/hour**	**mV/hour**	**m**
Units		**mbgl**	**mbgl**	**mbgl**										
AKEYO F.														
168	MSB-4	15.8	20.75	25.7				0.20	5.29	2				9.9
LOWER TOKI LIGNITE-BEARING FORMATION/TOKI GRANITE														
2	KNA-6 unconf.	-						0.1	-6.48	2				1.7678
LOWER TOKI LIGNITE-BEARING FORMATION														
165	MSB-2	132.0	142.99	154.0				1.8	-0.37	2	-0.006	-0.02	-1.2	22
TOKI GRANITE														
173	DH-2	305.6	306.55	307.6					-4.07	2				2
108	DH-7	560.5	563.75	567.0					-22.60	1	0.001	0.01	-0.4	6.5
151	DH-12	171.8	225.99	280.2				0.04	-2.20	2	0.00	0.01	-0.6	108.37
162	MIU-4	505.8	533.09	560.4				2.67	-0.05	2	0.002	0.01	0.6	54.65
166	MSB-2	171.5	173.49	175.5				2.25	-0.71	2	0.001	-0.12	-1	4
	MIZ-1	215.0	220.34	225.7				2.91	-5.74	2	0.02	0.04	9	10.67
	DH-15	437.6	449.85	462.1			0.338	33.80	1.96	2				24.5

Note: Yellow highlight indicates values calculated during the present work.

Table 5-1 continued.

Index	Location	Depth			Sampling location	Physico-chemical parameter measuring location	Pumping rate	Total extracted water volume	DO	log f $CO_2(g)$	Calcite saturation index	Calculated alkalinity (calculated from pH and TIC)	Reported Alkalinity
		Min	Middle	Max			Litres/minute	Litres	mg/L			meq/l	meq/l
Units		mbgl	mbgl	mbgl									
AKEYO F.													
168	MSB-4	15.8	20.75	25.7	2	3		583		-2.21	0.16	3.51	
LOWER TOKI LIGNITE-BEARING FORMATION/TOKI GRANITE													
2	KNA-6 unconf.	-			2	2							
LOWER TOKI LIGNITE-BEARING FORMATION													
165	MSB-2	132.0	142.99	154.0	2	2	4	11083	0.01	-4.52	0.0195	0.38	0.45
TOKI GRANITE													
173	DH-2	305.6	306.55	307.6	2	2				-4.24	0.1044	0.64	
108	DH-7	560.5	563.75	567.0	1	1	0.031	292		-5.39	0.94	3.63	1.51
151	DH-12	171.8	225.99	280.2	2	2	160	677698	0.01	-4.82	0.2	0.70	0.679
162	MIU-4	505.8	533.09	560.4	2	2	10	28000	0	-4.34	0.21	1.47	1.4
166	MSB-2	171.5	173.49	175.5	2	2	1.2	11700.1	0.01	-4.25	0.01	0.48	0.56
	MIZ-1	215.0	220.34	225.7	2	2	30	101826	0	-4.45	0.06	0.88	0.68
	DH-15	437.6	449.85	462.1	2	2		36601	0.00	-4.25	0.0756	0.58	0.57

Note: Yellow highlight indicates values calculated during the present work.

Table 5-2 Estimates of data quality based on the information given in Table 5-1.

Index	Location	Depth			pH (major cations, major anions, PA-relevant trace constituents)		Eh		Redox-sensitive trace elements		Inorganic carbon species	
		Min	Middle	Max	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)
Units		mbgl	mbgl	mbgl								
AKEYO F.												
168	MSB-4	15.8	20.75	25.7	0.52	0.24	0.01	0.00	0.01	0.00	0.54	0.24
TOKI LIGNITE BEARING F. (LOWER)												
2	KNA-6 unconf.	-			71	0.29	68	0.32	66	0.34	2.84	0.04
165	MSB-2	132.0	142.99	154.0	0.20	0.40	0.01	0.00	0.01	0.00	0.27	0.25
TOKI GRANITE												
173	DH-2	305.6	306.55	307.6	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
108	DH-7	560.5	563.75	567.0	0.02	0.50	0.02	0.50	0.02	0.50	0.02	0.50
151	DH-12	171.8	225.99	280.2	0.16	-0.16	0.05	-0.05	0.10	-0.10	0.22	-0.22
162	MIU-4	505.8	533.09	560.4	0.11	-0.11	0.01	0.00	0.01	0.00	0.16	-0.16
166	MSB-2	171.5	173.49	175.5	0.62	0.19	0.01	0.00	0.01	0.00	0.66	0.17
	MIZ-1	215.0	220.34	225.7	0.10	-0.10	0.01	0.00	0.01	0.00	0.06	-0.06
	DH-15	437.60	449.85	462.1	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00

Note: To avoid division of zero or division by zero, when calculating the ratio For/Against, any evidence values of zero are converted to a minimum of 0.01. This approach results in a possible ratio between 0.01 and 100. This approach is consistent with the approach adopted for plotting the ratio plot.

An important point is that the amount of quality information (number of different quality indicators) does not necessarily correlate with the residual uncertainty in a judgement. There was much more quality information available to the writer for the KNA-6 sample (Figure 5-1) than for the MSB-4 sample (Figure 3-11; more quality information exists but was not available to the writer). However, the judgement of pH quality in the former case has a higher residual uncertainty (0.31) than in the latter case (0.24). This difference reflects:

- the choice of sufficiency values;
- the fact that the level of support calculated by ESL for a given proposition (parent process) is not linearly dependent upon the number of supporting (child) processes, even when the sufficiencies of these child processes are the same.

This second point follows from the fact that 'evidence' or 'support' from different child processes for a given parent process overlap.

A process model to evaluate the quality of pH data for the interval between 132.0 m and 154.0 m depth in borehole MSB-2 is shown in Figure 5-2. This model illustrates that the large amount of water pumped during sampling, combined with the long test section and the observation that degassing occurred, results in a balance of evidence against the suitability of the data.

An evaluation of the quality of pH data for the interval between 305.6 m and 307.6 m depth in borehole DH-2 is shown in Figure 5-3. In this case the balance of 'evidence other than drilling fluid evidence' (Process 5) gives a small degree of support to the hypothesis that the pH value is of adequate quality. However, there is no information about the degree of drilling fluid contamination (Processes 3 and 4). Thus, the overall judgement of pH quality is completely uncertain.

In contrast the evaluation of pH quality for the interval between 560.5 m and 567.0 m in borehole DH-7 (Figure 5-4) indicates evidence against the pH's adequacy of 0.5, even though there is similarly no information about drilling fluid contamination.

These two results reflect the fact that if there is evidence for some data being adequate, in the absence of information about drilling fluid contamination, it cannot be stated whether the data are in fact adequate or not. On the other hand, if there is evidence that the data are inadequate, even if there is no information about drilling fluid contamination, the data must be inadequate.

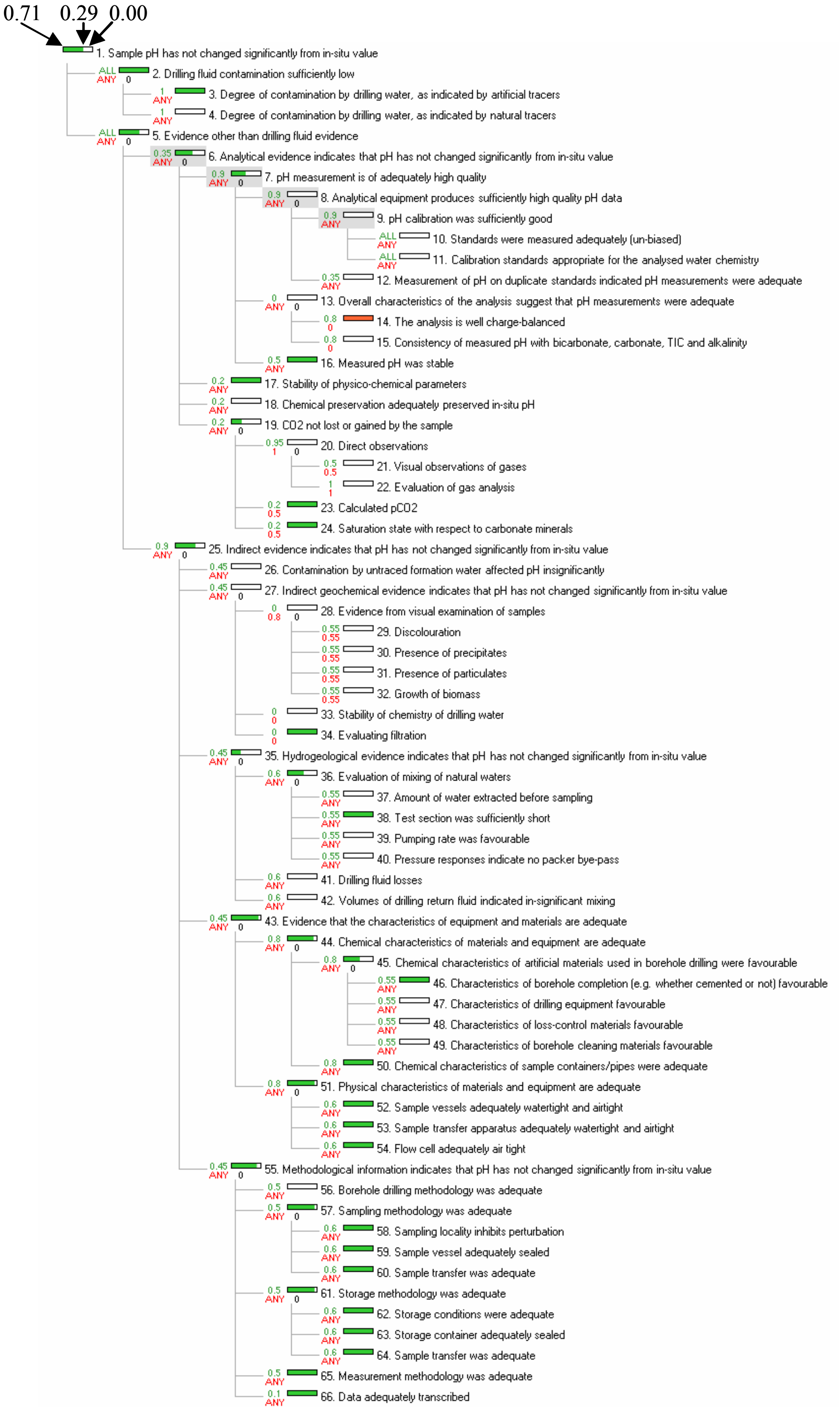


Figure 5-1 Process model showing an evaluation of the quality of pH data for water sampled from near the Toki Granite/Lower Toki Lignite-bearing Formation boundary in borehole KNA-6. In order to show the model on one page evidence values are given only for the top level process.

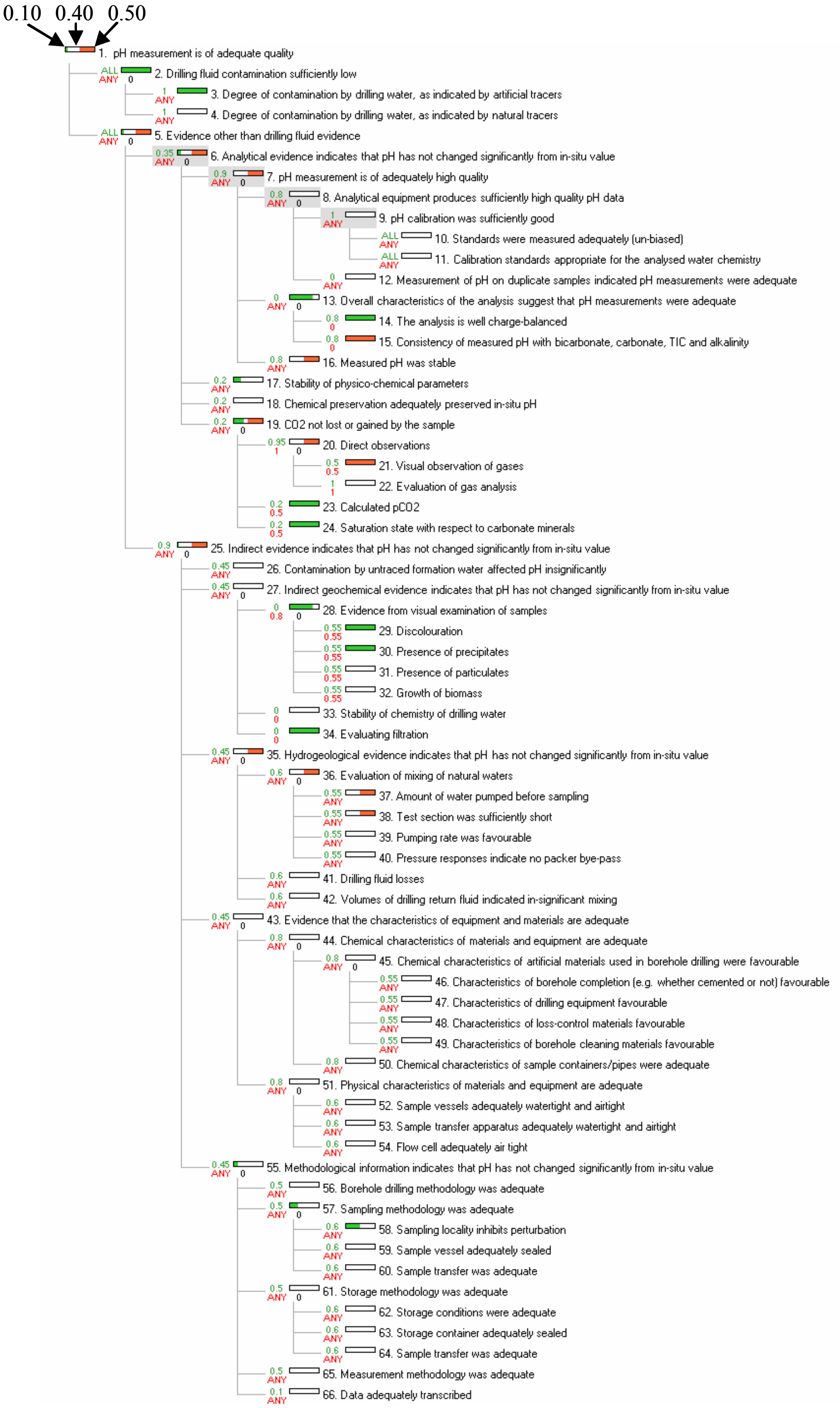


Figure 5-2 **A process model illustrating an evaluation of the quality of pH data for the interval between 132 m and 154 m depth in borehole MSB-2. In order to show the model on one page evidence values are given only for the top level process.**

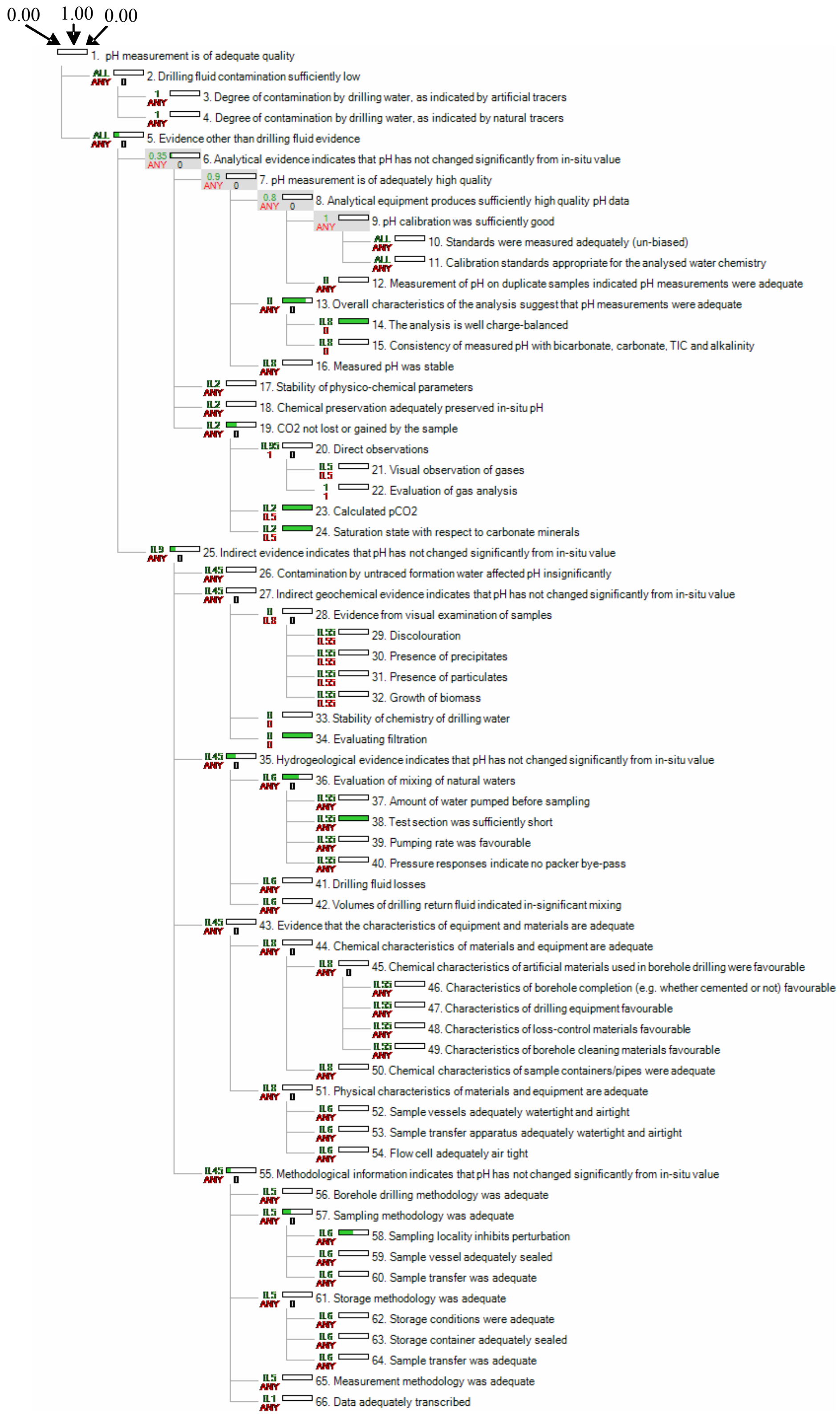


Figure 5-3 A process model illustrating an evaluation of the quality of pH data for the interval between 305.6 m and 307.6 m depth in borehole DH-2. In order to show the model on one page evidence values are given only for the top level process.

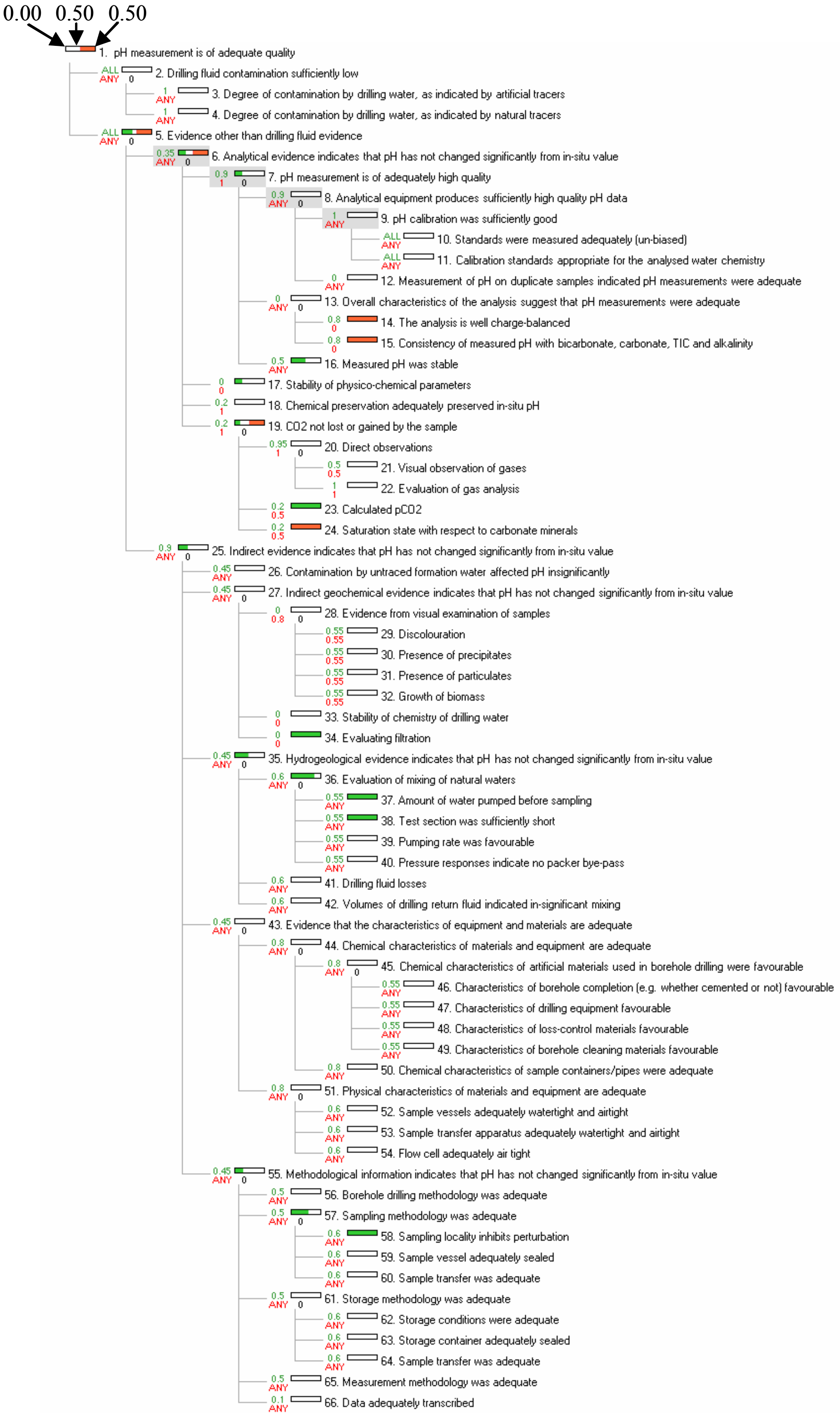


Figure 5-4 A process model illustrating an evaluation of the quality of pH data for the interval between 560.5 m and 567.0 m depth in borehole DH-7. In order to show the model on one page evidence values are given only for the top level process.

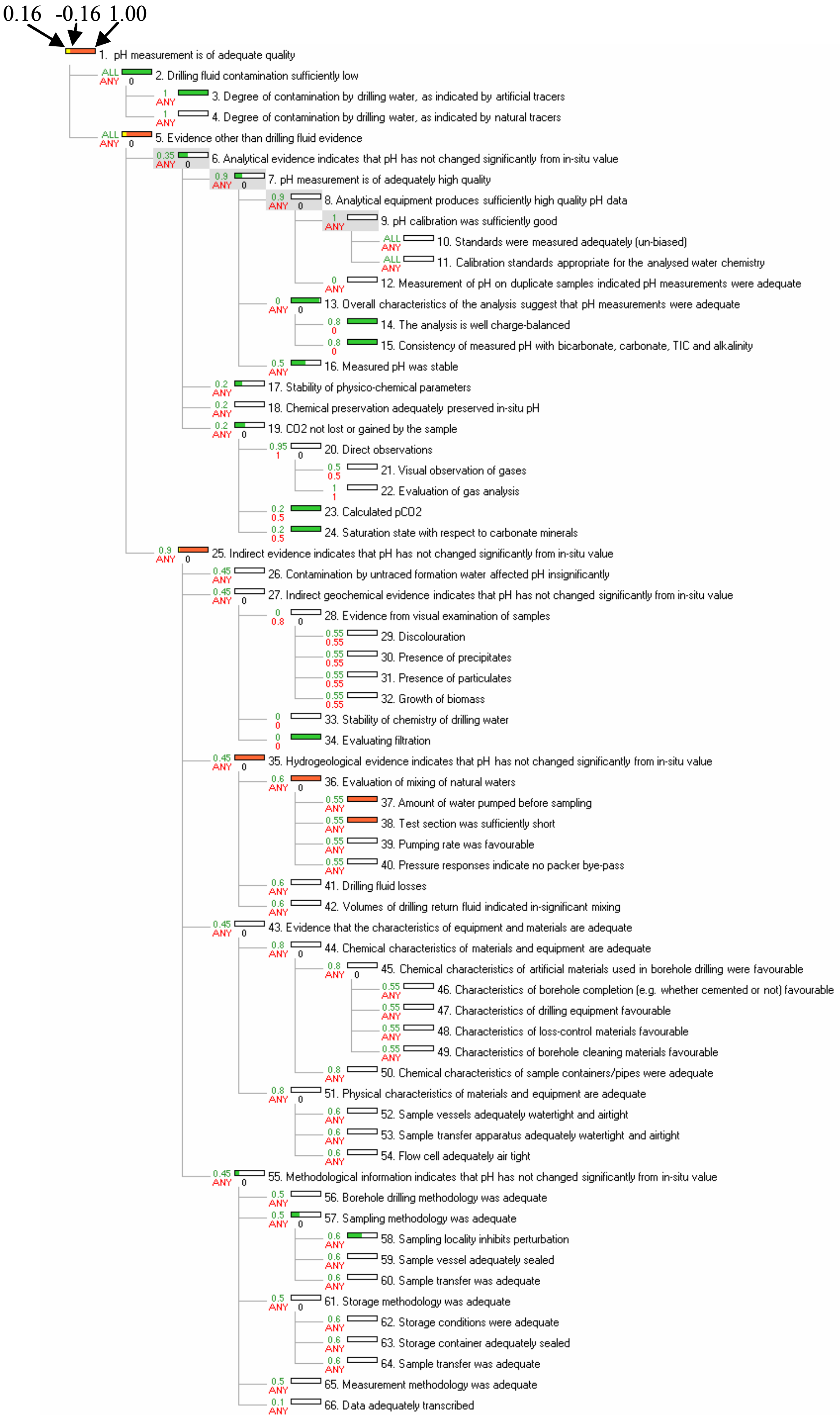


Figure 5-5 A process model illustrating an evaluation of the quality of pH data for the interval between 171.8 m and 280.2 m depth in borehole DH-12. In order to show the model on one page evidence values are given only for the top level process.

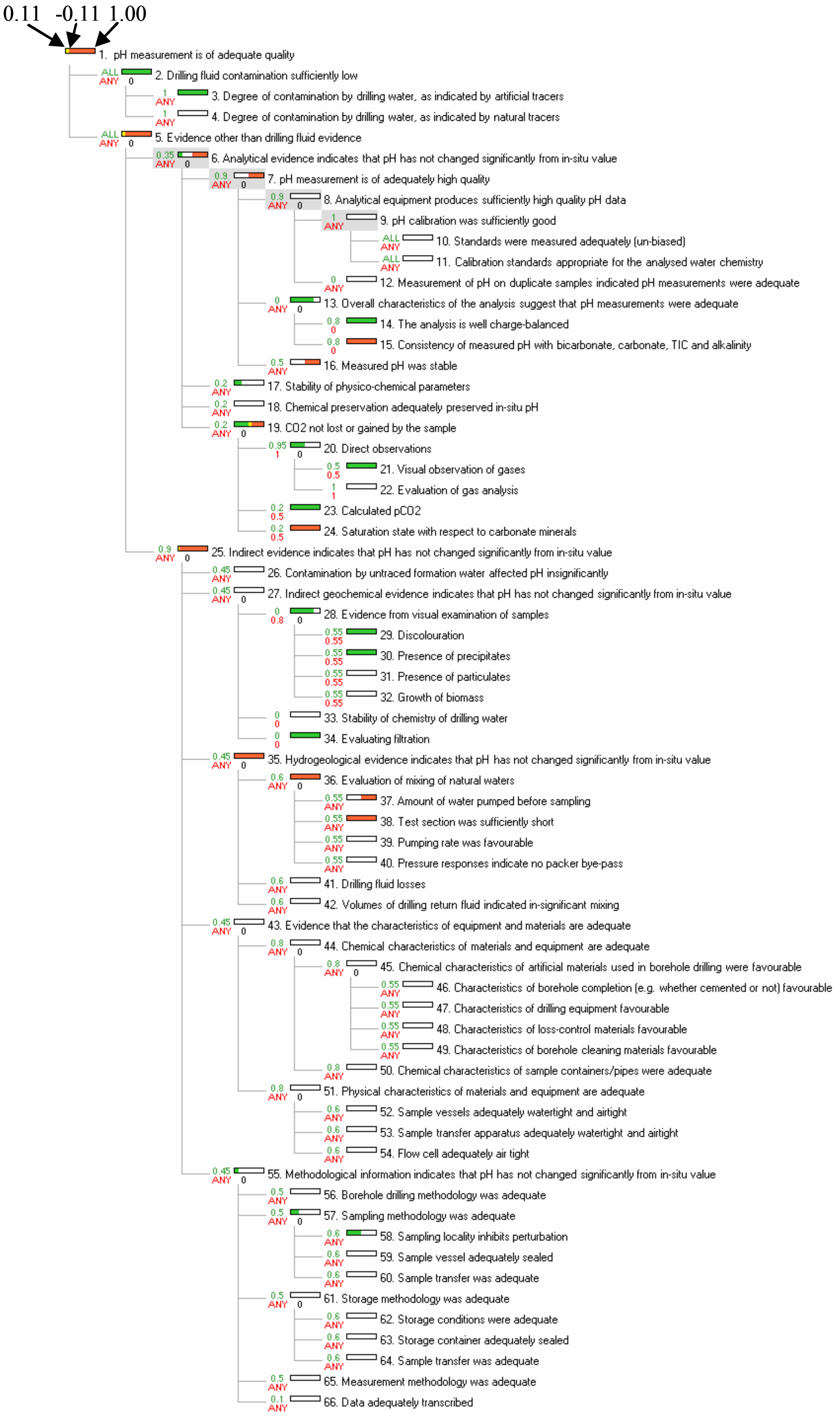


Figure 5-6 A process model illustrating an evaluation of the quality of pH data for the interval between 505.8 m and 560.4 m depth in borehole MIU-4. In order to show the model on one page evidence values are given only for the top level process.

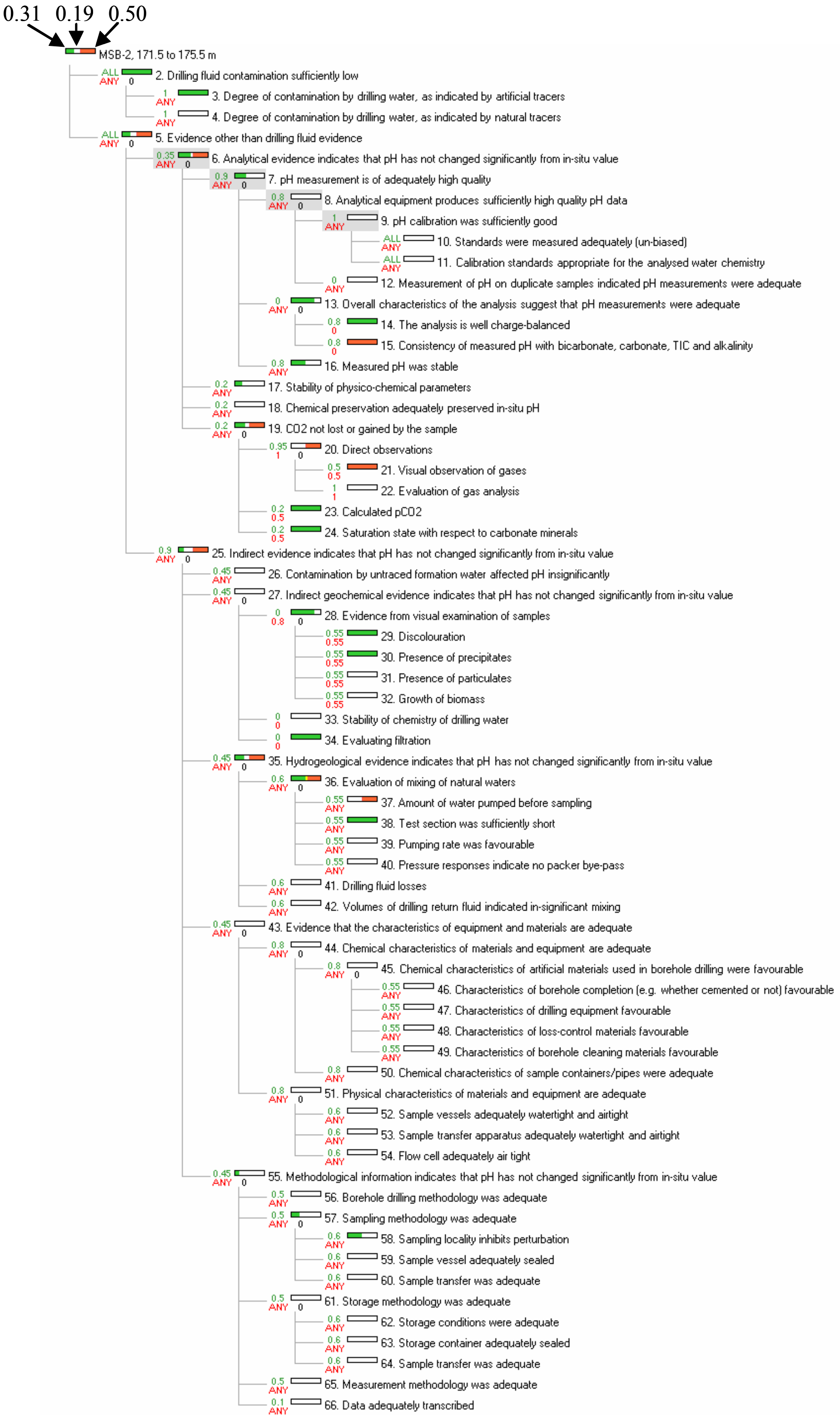


Figure 5-7 A process model illustrating an evaluation of the quality of pH data for the interval between 171.5 m and 175.5 m depth in borehole MSB-2. In order to show the model on one page evidence values are given only for the top level process.

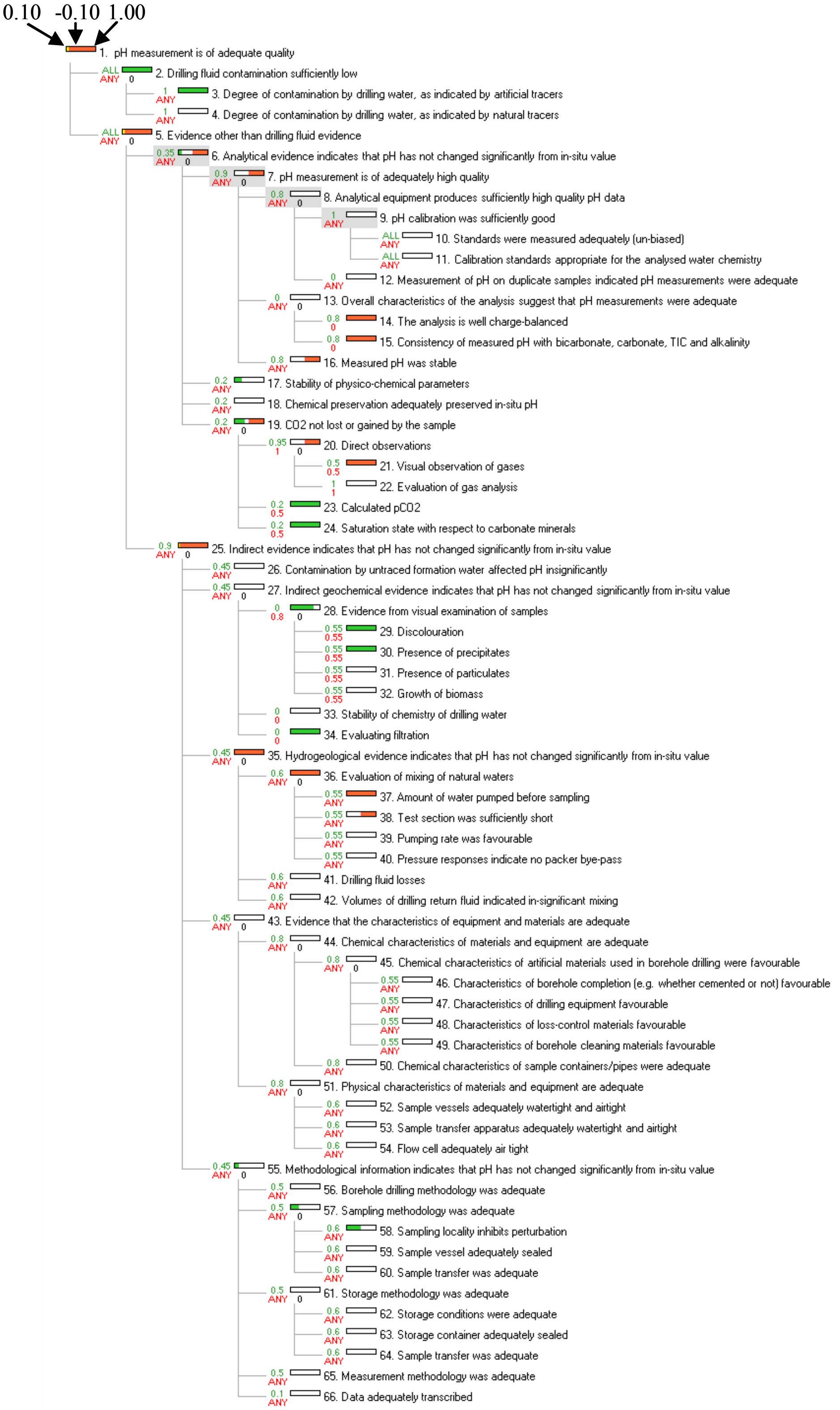


Figure 5-8 A process model illustrating an evaluation of the quality of pH data for the interval between 215.0 m and 225.7 m depth in borehole MIZ-1. In order to show the model on one page evidence values are given only for the top level process.

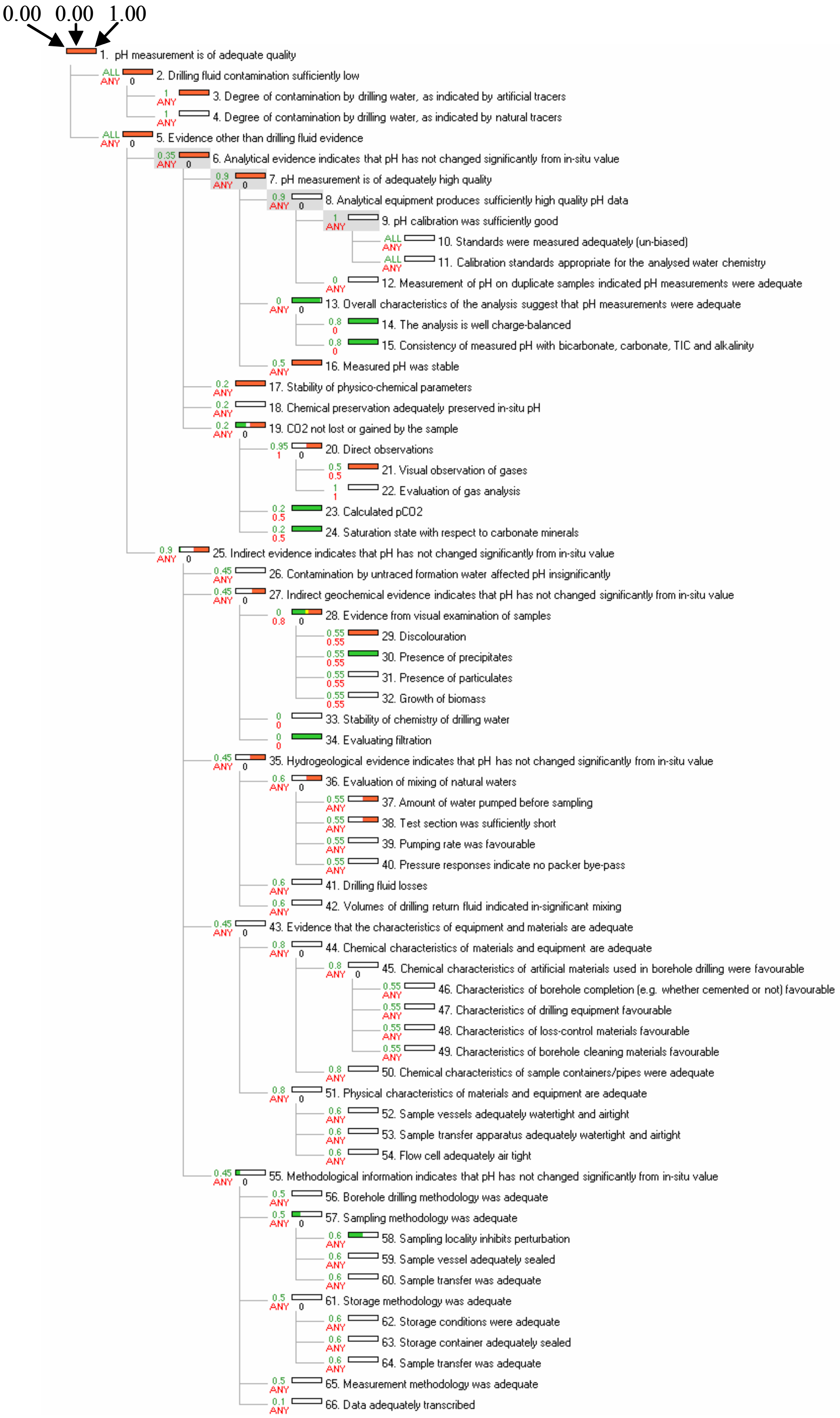


Figure 5-9 A process model illustrating an evaluation of the quality of pH data for the interval between 437.60 m and 462.1 m depth in borehole DH-15. In order to show the model on one page evidence values are given only for the top level process.

A convenient alternative way of comparing quality indicators for a particular sample, or comparing overall quality judgements made for different samples, is to employ a ratio plot (Figure 5-10). Such a plot displays the information presented in Table 5-2 in a graphical form, the evidence ratio ('evidence for'/'evidence against') being plotted on the vertical axis, and the residual uncertainty being plotted on the horizontal axis. Judgements where there is no conflicting evidence plot in the right hand half of the plot, whereas judgements. A conflict of evidence causes a judgement to plot in the left hand half of the plot. Each of these halves of the plots are divided into four fields, which indicate the degree to which a judgement is considered to be reliable.

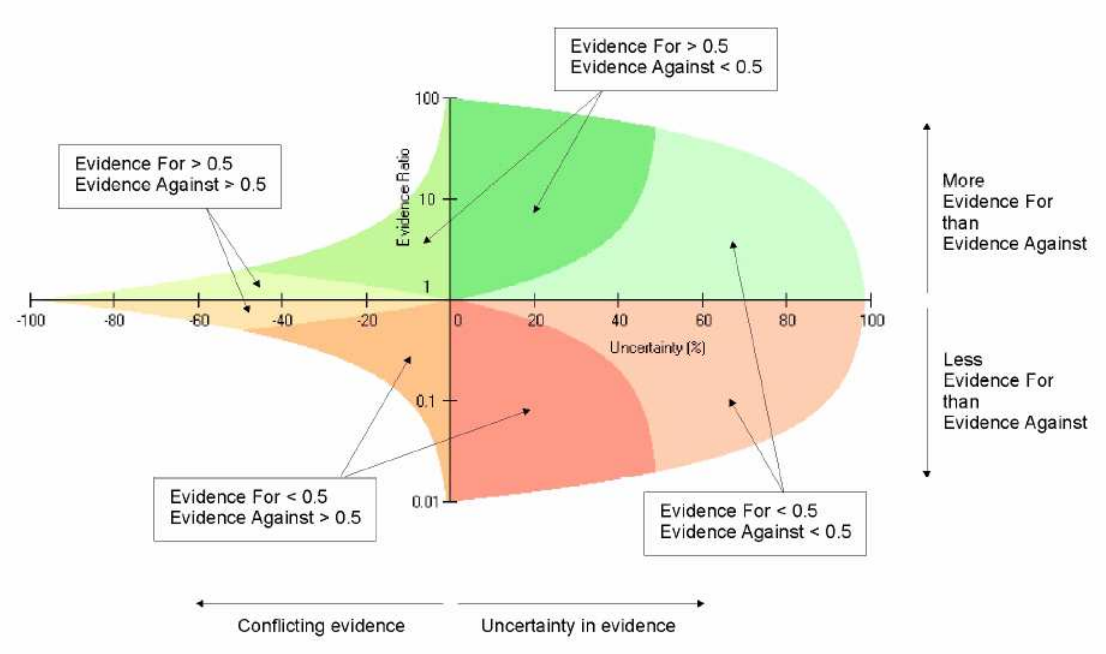
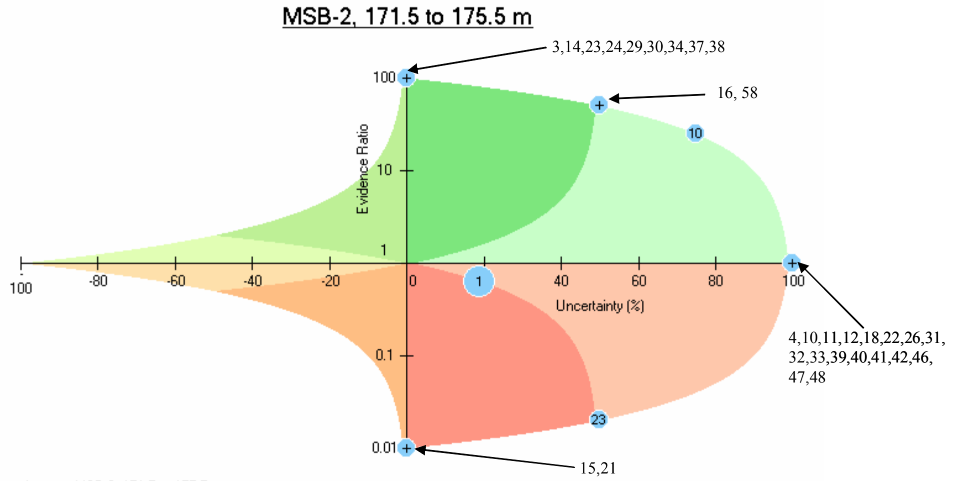


Figure 5-10 Example of a ratio plot, plotting the 'evidence ration ('evidence for'/'evidence against') against uncertainty. Values that plot in the dark green region are clearly indicated to be of adequate quality; values that plot in the light green region may be of adequate quality; values that plot in the dark red region are clearly indicated to be of inadequate quality and those in the light red region may be of inadequate quality.

As an illustration of the approach, the processes in Figure 5-7 (sample from MSB-2, between 171.5 and 175.5 m) are plotted on a ratio plot in Figure 5-11. This plot highlights that the pH value is deemed to be unreliable. However, a very small change in the evidence ratio would cause the pH value to be considered reliable. Such an up-graded judgement is within the range of variability allowed by the uncertainty.

The processes that contribute 'evidence for' and 'evidence against' the proposition that the pH value for this sample if of adequate quality plot in the top and bottom halves of the plot respectively.



1 : MSB-2, 171.5 to 175.5 m
2 : 3. Degree of contamination by drilling water, as indicated by artificial tracers
3 : 4. Degree of contamination by drilling water, as indicated by natural tracers
4 : 10. Standards were measured adequately (un-biased)
5 : 11. Calibration standards appropriate for the analysed water chemistry
6 : 12. Measurement of pH on duplicate samples indicated pH measurements were adequate
7 : 14. The analysis is well charge-balanced
8 : 15. Consistency of measured pH with bicarbonate, carbonate, TIC and alkalinity
9 : 16. Measured pH was stable
10 : 17. Stability of physico-chemical parameters
11 : 18. Chemical preservation adequately preserved in-situ pH
12 : 21. Visual observation of gases
13 : 22. Evaluation of gas analysis
14 : 23. Calculated pCO2
15 : 24. Saturation state with respect to carbonate minerals
16 : 26. Contamination by untraced formation water affected pH insignificantly
17 : 29. Discolouration
18 : 30. Presence of precipitates
19 : 31. Presence of particulates
20 : 32. Growth of biomass
21 : 33. Stability of chemistry of drilling water
22 : 34. Evaluating filtration
23 : 37. Amount of water pumped before sampling
24 : 38. Test section was sufficiently short
25 : 39. Pumping rate was favourable
26 : 40. Pressure responses indicate no packer bye-pass
27 : 41. Drilling fluid losses
28 : 42. Volumes of drilling return fluid indicated in-significant mixing
29 : 46. Characteristics of borehole completion (e.g. whether cemented or not) favourable
30 : 47. Characteristics of drilling equipment favourable
31 : 48. Characteristics of loss-control materials favourable
32 : 49. Characteristics of borehole cleaning materials favourable
33 : 50. Chemical characteristics of sample containers/pipes were adequate
34 : 52. Sample vessels adequately watertight and airtight
35 : 53. Sample transfer apparatus adequately watertight and airtight
36 : 54. Flow cell adequately air tight
37 : 56. Borehole drilling methodology was adequate
38 : 58. Sampling locality inhibits perturbation
39 : 59. Sample vessel adequately sealed
40 : 60. Sample transfer was adequate
41 : 62. Storage conditions were adequate
42 : 63. Storage container adequately sealed
43 : 64. Sample transfer was adequate
44 : 65. Measurement methodology was adequate
45 : 66. Data adequately transcribed

Figure 5-11 Comparison of evidence for the various process in Figure 5-7 using a ratio plot.

Processes for which there is no corresponding quality information plot at the right hand extremity of the horizontal axis.

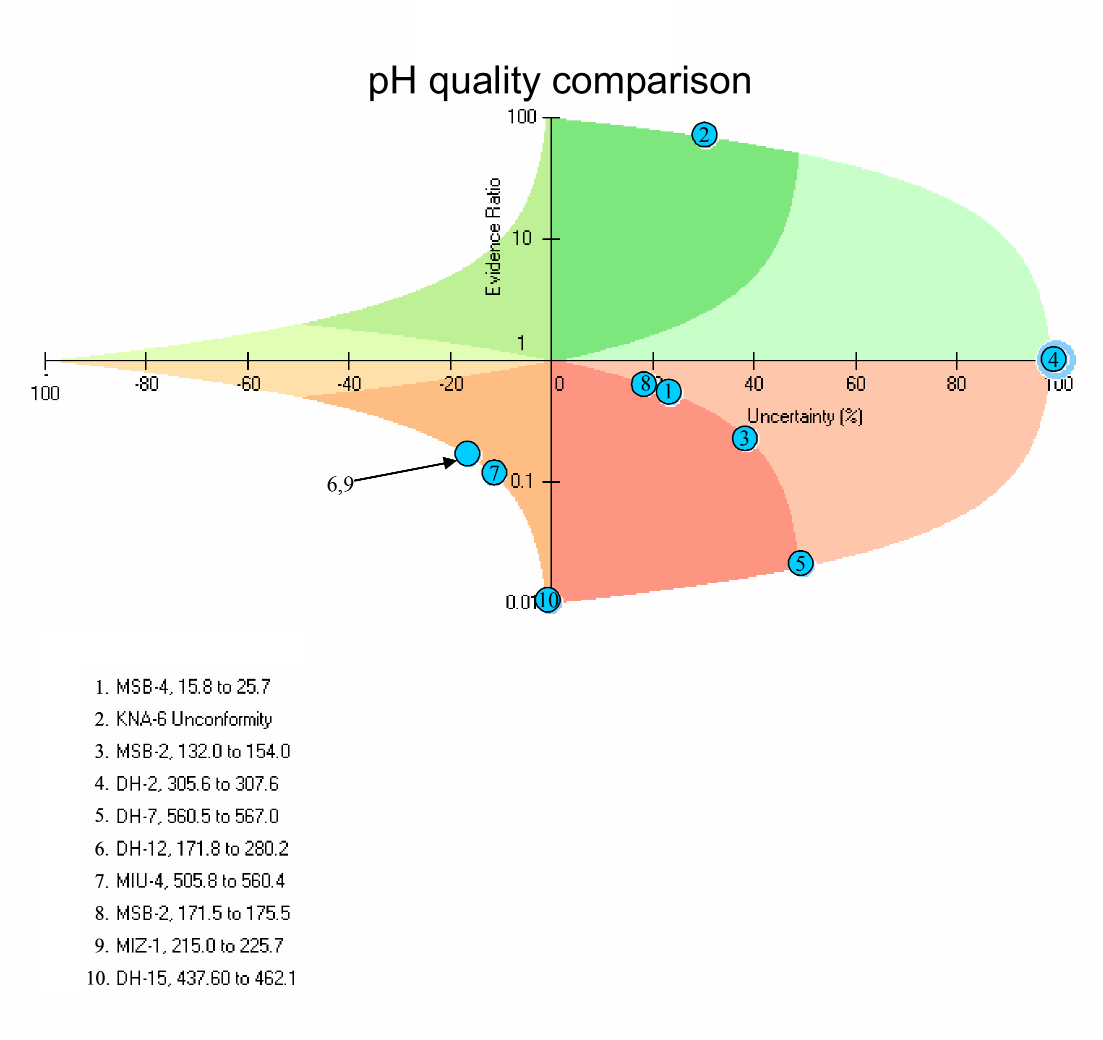


Figure 5-12 Comparison of the quality of pH data presented in Figure 3-11 and Figure 5-1 to Figure 5-9.

The judgements of pH data quality illustrated in Figure 3-11 and Figure 5-1 to Figure 5-9 are compared using a ratio plot in Figure 5-12. This figure illustrates that only the data obtainted from KNA-6 (Figure 5-1) are considered to be clearly reliable. This result reflects the fact that the data from KNA-6 were obtained during long-term monitoring. However, it is noted that there was no information available concerning the amount of water extracted during data acquisition (Process 37). If data became available that indicated large amounts of water were extracted, causing significant mixing of in-situ water, the result would be a conflict of evidence. The judgement would then plot in the upper left hand quadrant of the figure, near to the horizontal axis.

The samples from MSB-4 (1; 15.8 m to 25.7 m), MSB-2 (3; 132.0 m to 154.0 m), DH-7 (5; 560.5 m to 567.0 m), and MSB-2 (8; 171.5 m to 175.5 m) all plot along the boundary between the dark and light red fields of the ratio plot. These pH data are all deemed to be of inadequate quality. Major causes of this inadequacy are:

- the measurement methodology (lab measurement) for the MSB-4 sample (Figure 3-11)
- visual observation of gases, amount of pumped water and length of test section for the MSB-2 sample from between 132.0 and 154.0 m (Figure 5-2);
- saturation state with respect to carbonate minerals for the DH-7 sample (Figure 5-4);
- visual observation of gases in the MSB-2 sample from between 171.5 m and 175.5 m (Figure 5-7).

In the case of the sample from MSB-2 between 132.0 m and 154.0 m depth, the amount of pumped water and the length of the test section are major contributors to inadequate data quality. However, as noted in 4.2.2 , the criteria adopted in the present work for setting ‘evidence for’ and ‘evidence against’ values are uncertain. If a more rigorous evaluation showed that the pumped water volume and test section length were more favourable, then the judgement of the pH data quality could also change favourable.

This illustrates how the data classification methodology may be used to identify the causes of poor data quality. In cases where an evaluation of poor quality results from a lack of information, then steps can be taken to improve the information available. Improvements can either involve processing existing data more appropriately, or else obtaining new information.

The samples from DH-12 (6; 171.8 m to 280.2 m), MIU-4 (7; 505.8 m to 560.4 m) and MIZ-1 (9; 215.0 m to 225.7 m) plot in the lower quadrant of the left hand side of the plot (Figure 5-12). Each of these samples produces a conflict between chemical data that indicates the pH value may be of adequate quality, and information concerning the length of the sampled section and the amount of water pumped that suggest the pH data may be inadequate. Once again, this judgement depends largely upon the criteria that are chosen to evaluate the possibility of groundwater mixing during sampling.

The pH value of the sample from DH-15 (10; 437.60 m to 462.1 m) is clearly of inadequate quality. This judgement follows not only from an appraisal of hydrogeological information, but also from a consideration of chemical information.

It is noted that these judgements of data quality relate to the adequacy of the data as they are reported. They do not preclude the possibility that in many cases corrections can be made for the processes that may have affected data quality. For example, calcite is over-saturated in the sample from from DH-7 between 560.5 m to 567.0 m, leading to the conclusion that CO_2 has probably degassed during sampling, affecting the pH adversely. However, it would be possible to correct for this CO_2 loss, assuming that the in-situ water is equilibrated with calcite. Such a correction procedure is in fact commonly carried out.

6 Conclusions: potential applications of the quality classification methodology

The quality classification methodology described in this report enables the quality of a geochemical parameter to be represented by two numerical quantities:

- the ratio of 'evidence for' to 'evidence against' (0.20 in the example shown in Figure 5-2);
- the residual uncertainty (0.40 in the example shown in Figure 5-2).

To prevent division by zero, if there is no 'evidence against', then a limiting value of 0.01 is taken. This would result in a quality index of 69.00 for the pH data from KNA-6 illustrated in Figure 5-1. However, the residual uncertainty in this case is very high, 0.31.

The quality classification methodology may be used to:

- rank samples, according to their 'evidence ratios';
- rank samples according to the degrees of uncertainty concerning data quality;
- highlight analyses that are clearly unsuitable for use in PA and SA;
- highlight samples that may be suitable for PA and SA;
- determine the main causes of uncertainty in data quality.

The appraisal of existing data illustrates that much of it is of apparently inadequate quality. However, this judgement must be qualified by two important points:

- There is considerable uncertainty concerning the importance of physical hydrogeological processes perturbing the in-situ groundwater chemistry. The present work used a highly simplified approach for choosing judgement criteria for hydrogeological parameters. This was done in order to illustrate the methodology. A more rigorous appraisal needs to be made on a test-by-test basis, taking into account the many processes that could affect mixing and consequently groundwater chemistry.

- ▲ The methodology evaluated only the adequacy of the data as they are reported. It did not consider the possibility that many of the processes causing perturbations to analysed parameters may be corrected by theoretical modelling.

If future developments of the methodology take these points into account it is expected that many more data will be considered to be of adequate quality.

By highlighting that uncertainty exists and also identifying the causes of uncertainty, the methodology can be used as a planning tool to set priorities for future investigations. Alternatively, it may highlight the need to search existing documentary records for additional quality information that may have been obtained initially but not reported together with the analyses.

The process models provide a visualisation of data quality judgements that may be appraised rapidly. The models can be revised readily as and when additional quality information becomes available, or to reflect the differing opinions of different experts concerning data quality.

It is suggested that the process models should be reviewed and revised as necessary by different experts, so as to build a consensus about what levels of data quality are desirable and attainable.

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Appendix 1 Summary of the availability of quality information used by JNC in H15 to calculate quality scores for groundwater compositions

Table A1-1 Summary of data quality classified according to JNC's H15 system.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
SETO GROUP															
38	N.R.	N.R.	N.R.	N.R.	N.R.	2.32	N.I.	0.07	0.25	N.I.	N.I.	N.I.	N.I.	1.00	1.00
37, 42	N.R.	N.R.	N.R.	N.R.	N.R.	0.57	N.I.	0.32	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
MIZUNAMI GROUP															
39	N.R.	N.R.	N.R.	N.R.	N.R.	0.36	N.I.	0.11	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
40	N.R.	N.R.	N.R.	N.R.	N.R.	0.91	N.I.	0.66	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
OIDAWARA F.															
13	TH-6	68.00	246.50	246.20	N.R.	2.29	N.I.	0.70	0.25	N.I.	N.I.	N.I.	0.00	1.00	0.33
14	TH-8	28.50	N.R.	247.30	N.R.	2.70	N.I.	0.97	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
43	N.R.	N.R.	N.R.	N.R.	N.R.	0.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
47	Avg.	N.R.	N.R.	N.R.	N.R.	1.00	N.I.	1.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
94	TH-8	28.50	N.R.	247.30	N.R.	2.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	1.00	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
OIDAWARA F.															
95	TH-6	68.00	N.R.	246.50	N.R.	2.22	N.I.	0.63	0.25	N.I.	N.I.	N.I.	N.I.	1.00	0.33
N.G.	DH-11	132.00	135.40	207.88	204.48	3.75	0.02	0.32	1.00	0.07	0.10	0.04	0.21	1.00	1.00
AKEYO F.															
15	TH-1	33.80	N.R.	253.20	N.R.	2.72	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
16	TH-2	32.80	N.R.	257.40	N.R.	2.58	N.I.	0.86	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
17	TH-3	46.50	N.R.	252.10	N.R.	2.08	N.I.	0.36	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
18	TH-4	61.00	N.R.	248.90	N.R.	2.33	N.I.	0.61	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
19	TH-6	104.00	N.R.	210.50	N.R.	2.02	N.I.	0.30	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
230	TH-6	104.00	N.R.	210.50	N.R.	2.09	N.I.	0.37	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
20	TH-8	64.00	N.R.	211.80	N.R.	2.09	N.I.	0.37	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
97	TH-8	64.00	N.R.	211.80	N.R.	2.25	N.I.	0.53	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
21	AN-6	14.00	N.R.	240.10	N.R.	2.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	1.00	0.33
96	AN-6	14.00	N.R.	240.10	N.R.	2.11	N.I.	0.53	0.25	N.I.	N.I.	N.I.	N.I.	1.00	0.33
48	Avg.	N.R.	N.R.	N.R.	N.R.	1.00	N.I.	1.00		N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
168	MSB-4	15.80	25.70	198.70	188.80	2.61	1.00	0.46	0.25	N.I.	N.I.	N.I.	0.07	0.50	0.33
169	MSB-4	34.80	62.20	179.70	152.30	2.61	1.00	0.50	0.25	N.I.	N.I.	N.I.	0.03	0.50	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
AKEYO F.															
N.G.	MSB-4	15.80	25.70	198.70	188.80	3.15	1.00	1.00	0.25	N.I.	N.I.	N.I.	0.07	0.50	0.33
N.G.	MSB-4	26.50	33.90	188.00	180.60	2.67	1.00	0.49	0.25	N.I.	N.I.	N.I.	0.09	0.50	0.33
N.G.	MSB-4	34.80	62.20	179.70	152.30	3.00	1.00	0.89	0.25	N.I.	N.I.	N.I.	0.03	0.50	0.33
N.G.	DH-15	63.00	72.50	N.R.	N.R.	4.07	1.00	1.00	1.00	0.05	0.10	0.01	0.07	0.50	0.33
N.G.	DH-15	84.50	97.50	N.R.	N.R.	3.77	0.48	1.00	1.00	0.20	0.20	0.01	0.05	0.50	0.33
TOKI LIGNITE BEARING F. (UPPER)															
44	N.R.	N.R.	N.R.	N.R.	N.R.	0.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
22	TH-1	70.80	N.R.	216.20	N.R.	2.27	N.I.	0.54	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
23	TH-2	74.80	N.R.	215.40	N.R.	2.72	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
24	TH-3	85.50	N.R.	213.10	N.R.	2.72	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
25	TH-4	83.00	N.R.	226.90	N.R.	2.34	N.I.	0.61	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
26	TH-6	132.00	N.R.	182.50	N.R.	2.36	N.I.	0.64	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
231	TH-6	132.00	N.R.	182.50	N.R.	2.16	N.I.	0.44	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
27	TH-8	91.00	N.R.	185.10	N.R.	2.31	N.I.	0.59	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI LIGNITE BEARING F. (UPPER)															
49	Avg.	N.R.	N.R.	N.R.	N.R.	0.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
152	DH 13	10.50	20.55	267.01	256.96	4.07	1.00	1.00	1.00	N.I.	N.I.	N.I.	0.07	0.50	0.50
TOKI LIGNITE BEARING F. (LOWER)															
28	TH-1	138.30	N.R.	148.10	N.R.	1.85	N.I.	0.13	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
29	TH-2	109.80	N.R.	179.50	N.R.	2.72	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
30	TH-3	124.00	N.R.	173.60	N.R.	2.72	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
31	TH-4	152.50	N.R.	157.60	N.R.	1.89	N.I.	0.17	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
98	TH-4	152.20	N.R.	157.70	N.R.	2.11	N.I.	0.39	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
32	TH-6	153.00	N.R.	159.80	N.R.	2.04	N.I.	0.32	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
232	TH-6	153.00	N.R.	159.80	N.R.	1.79	N.I.	0.07	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
33	TH-8	121.00	N.R.	155.10	N.R.	2.72	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
41						0.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
1	KNA-6 sed.	N.R.	N.R.	143.00	N.R.	4.24	1.00	1.00	0.25	N.I.	N.I.	N.I.	0.99	0.50	0.50

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI LIGNITE BEARING F. (LOWER)															
2	KNA-6 unconf.	N.R.	N.R.	136.00	N.R.	3.65	1.00	1.00	0.25	N.I.	N.I.	N.I.	0.40	0.50	0.50
3	KNA-6 gra.	N.R.	N.R.	121.00	N.R.	2.88	1.00	0.61	0.25	N.I.	N.I.	N.I.	0.02	0.50	0.50
46	KNA-2	153.00	N.R.	N.R.	N.R.	1.25	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	0.50	0.50
45	N.R.	N.R.	N.R.	N.R.	N.R.	0.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
50	Avg.	N.R.	N.R.	N.R.	N.R.	0.00	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.	N.I.
52	TFA-1	14.60	14.79	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
53	TFA-1	14.79	15.04	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
54	TFA-1	15.04	15.30	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
150	DH-12	157.45	164.12	-20.07	-26.74	4.32	1.00	1.00	1.00	0.01	0.20	0.00	0.10	0.50	0.50
159	MIU-4	71.45	76.77	145.54	140.22	4.54	1.00	1.00	1.00	0.20	0.20	0.01	0.13	0.50	0.50
164	MSB-2	79.00	130.49	119.49	68.00	4.00	0.59	0.97	1.00	0.20	0.20	0.03	0.01	0.50	0.50
165	MSB-2	131.99	153.99	66.50	44.50	3.74	0.56	1.00	1.00	0.03	0.10	0.02	0.03	0.50	0.50
TOKI GRANITE															
34	TH-1	166.30	N.R.	120.10	N.R.	1.92	N.I.	0.20	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
35	TH-6	177.50	N.R.	135.30	N.R.	1.95	N.I.	0.23	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
		Min.	Max.	Min.	Max.	OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
							Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI GRANITE															
233	TH-6	177.50	N.R.	135.30	N.R.	2.44	N.I.	0.71	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
105	TH-8	160.00	N.R.	115.80	N.R.	2.49	N.I.	0.77	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
N.G.	TH-8	N.R.	N.R.	N.R.	N.R.	1.72	N.I.	-	0.25	N.I.	N.I.	N.I.	0.14	1.00	0.33
170	DH-2	207.50	209.50	-13.87	-15.87	2.20	N.I.	0.60	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
171	DH-2	228.50	237.00	-34.87	-43.37	1.58	N.I.	0.25	0.25	N.I.	N.I.	N.I.	0.08	0.50	0.50
172	DH-2	302.70	304.70	-109.07	-111.07	2.60	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
173	DH-2	305.55	307.55	-111.92	-113.92	2.01	N.I.	0.41	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
174	DH-2	309.70	311.70	-116.07	-118.07	2.25	N.I.	0.65	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
175	DH-2	313.00	315.00	-119.37	-121.37	2.60	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
176	DH-2	320.90	328.40	-127.27	-134.77	2.26	N.I.	0.91	0.25	N.I.	N.I.	N.I.	0.09	0.50	0.50
177	DH-2	347.80	349.80	-154.17	-156.17	2.60	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
178	DH-2	365.50	367.50	-171.87	-173.87	1.95	N.I.	0.35	0.25	N.I.	N.I.	N.I.	0.35	0.50	0.50
179	DH-2	439.50	448.00	-245.87	-254.37	1.84	N.I.	0.51	0.25	N.I.	N.I.	N.I.	0.08	0.50	0.50
180	DH-2	451.20	459.70	-257.57	-266.07	1.95	N.I.	0.61	0.25	N.I.	N.I.	N.I.	0.08	0.50	0.50
51	DH-3	0.00	0.00	356.40	356.40	1.79	N.I.	0.21	0.25	N.I.	N.I.	N.I.	N.I.	1.00	0.33
N.G.	DH-3	19.10	25.40	337.30	331.00	1.69	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI GRANITE															
N.G.	DH-3	129.80	138.90	226.60	217.50	1.66	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	0.08	1.00	0.33
220	DH-3	129.80	138.90	226.60	217.50	2.66	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.08	1.00	0.33
6	DH-3	206.80	218.90	149.60	137.50	1.70	N.I.	0.06	0.25	N.I.	N.I.	N.I.	0.06	1.00	0.33
221	DH-3	206.80	218.90	149.60	137.50	1.67	N.I.	0.03	0.25	N.I.	N.I.	N.I.	0.06	1.00	0.33
7	DH-3	325.20	332.10	31.20	24.30	1.74	N.I.	0.06	0.25	N.I.	N.I.	N.I.	0.10	1.00	0.33
222	DH-3	325.20	332.10	31.20	24.30	1.77	N.I.	0.08	0.25	N.I.	N.I.	N.I.	0.10	1.00	0.33
N.G.	DH-3	458.50	466.70	-102.10	-110.30	1.67	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	0.09	1.00	0.33
223	DH-3	458.50	466.70	-102.10	-110.30	1.81	N.I.	0.14	0.25	N.I.	N.I.	N.I.	0.09	1.00	0.33
8	DH-3	486.50	498.40	-130.10	-142.00	1.69	N.I.	0.05	0.25	N.I.	N.I.	N.I.	0.06	1.00	0.33
224	DH-3	486.50	498.40	-130.10	-142.00	1.81	N.I.	0.17	0.25	N.I.	N.I.	N.I.	0.06	1.00	0.33
N.G.	DH-3	601.20	613.40	-244.80	-257.00	1.71	N.I.	0.07	0.25	N.I.	N.I.	N.I.	0.06	1.00	0.33
225	DH-3	601.20	613.40	-244.80	-257.00	1.86	N.I.	0.22	0.25	N.I.	N.I.	N.I.	0.06	1.00	0.33
9	DH-3	641.10	648.60	-284.70	-292.20	1.68	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	0.09	1.00	0.33
226	DH-3	641.10	648.60	-284.70	-292.20	2.43	N.I.	0.75	0.25	N.I.	N.I.	N.I.	0.09	1.00	0.33
227	DH-3	767.00	774.50	-410.60	-418.10	1.79	N.I.	0.12	0.25	N.I.	N.I.	N.I.	0.09	1.00	0.33
10	DH-3	790.70	797.90	-434.30	-441.50	1.76	N.I.	0.08	0.25	N.I.	N.I.	N.I.	0.10	1.00	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI GRANITE															
228	DH-3	790.70	797.90	-434.30	-441.50	2.14	N.I.	0.46	0.25	N.I.	N.I.	N.I.	0.10	1.00	0.33
11	DH-3	829.10	837.40	-472.70	-481.00	1.75	N.I.	0.08	0.25	N.I.	N.I.	N.I.	0.08	1.00	0.33
229	DH-3	829.10	837.40	-472.70	-481.00	2.14	N.I.	0.47	0.25	N.I.	N.I.	N.I.	0.08	1.00	0.33
5	DH-4	185.50	188.50	81.08	78.08	3.57	N.I.	1.00	1.00	N.I.	N.I.	N.I.	0.23	1.00	0.33
106 4)	DH-5	323.80	330.80	-13.35	-20.35	4.23	N.I.	1.00	1.00	0.03	0.09	0.01	0.10	1.00	1.00
107	DH-6	733.00	740.00	-413.70	-420.70	4.23	N.I.	1.00	1.00	0.03	0.05	0.05	0.10	1.00	1.00
N.G.	DH-7	438.00	444.50	-97.81	-104.31	2.69	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	479.00	485.50	-138.81	-145.31	2.53	N.I.	0.84	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	479.00	485.50	-138.81	-145.31	2.39	N.I.	0.70	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
108	DH-7	560.50	567.00	-220.31	-226.81	3.73	N.I.	0.17	1.00	0.20	0.20	0.05	0.11	1.00	1.00
N.G.	DH-7	560.50	567.00	-220.31	-226.81	2.13	N.I.	0.44	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	560.50	567.00	-220.31	-226.81	2.21	N.I.	0.52	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	598.00	604.50	-257.81	-264.31	2.13	N.I.	0.44	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	598.00	604.50	-257.81	-264.31	1.92	N.I.	0.23	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	660.00	666.50	-319.81	-326.31	2.17	N.I.	0.48	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	660.00	666.50	-319.81	-326.31	1.94	N.I.	0.25	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
							Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.	OVERALL QUALITY SCORE	Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI GRANITE															
N.G.	DH-7	735.50	742.00	-395.31	-401.81	2.29	N.I.	0.60	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	735.50	742.00	-395.31	-401.81	1.98	N.I.	0.29	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
109	DH-7	833.50	840.00	-493.31	-499.81	3.58	N.I.	0.14	1.00	0.10	0.20	0.03	0.11	1.00	1.00
N.G.	DH-7	833.50	840.00	-493.31	-499.81	2.69	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
110	DH-7	880.00	886.50	-539.81	-546.31	3.58	N.I.	0.23	1.00	0.20	0.03	0.01	0.11	1.00	1.00
N.G.	DH-7	880.00	886.50	-539.81	-546.31	2.20	N.I.	0.51	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
N.G.	DH-7	880.00	886.50	-539.81	-546.31	1.92	N.I.	0.23	0.25	N.I.	N.I.	N.I.	0.11	1.00	0.33
111	DH-8	641.50	648.00	-371.68	-378.18	3.95	N.I.	0.53	1.00	0.20	0.10	0.01	0.11	1.00	1.00
112	DH-8	693.50	700.00	-423.68	-430.18	3.57	N.I.	0.15	1.00	0.10	0.20	0.02	0.11	1.00	1.00
113	DH-8	745.50	752.00	-475.68	-482.18	3.34	N.I.	0.18	1.00	0.03	0.02	0.00	0.11	1.00	1.00
114	DH-8	869.00	875.50	-599.18	-605.68	3.87	N.I.	0.36	1.00	0.20	0.20	0.00	0.11	1.00	1.00
115	DH-8	975.00	981.50	-705.18	-711.68	3.67	N.I.	0.23	1.00	0.20	0.10	0.03	0.11	1.00	1.00
N.G.	DH-9	228.00	234.50	47.42	40.92	4.56	N.I.	1.00	1.00	0.20	0.20	0.05	0.11	1.00	1.00
N.G.	DH-9	312.90	319.40	-37.48	-43.98	3.86	N.I.	0.24	1.00	0.16	0.20	0.16	0.11	1.00	1.00
N.G.	DH-9	957.30	963.80	-681.88	-688.38	4.06	N.I.	0.39	1.00	0.16	0.20	0.20	0.11	1.00	1.00
N.G.	DH-10	333.50	341.50	142.06	134.06	4.13	0.13	0.51	1.00	0.20	0.20	0.01	0.09	1.00	1.00

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI GRANITE															
N.G.	DH-10	46.50	61.50	429.06	414.06	2.13	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.05	0.50	0.33
N.G.	DH-10	46.50	121.50	429.06	354.06	1.92	N.I.	0.83	0.25	N.I.	N.I.	N.I.	0.01	0.50	0.33
N.G.	DH-11	392.50	468.00	-52.62	-128.12	2.09	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.01	0.50	0.33
N.G.	DH-11	932.00	1007.50	-592.12	-667.62	2.09	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.01	0.50	0.33
151	DH-12	171.80	280.17	-34.42	-142.79	4.01	1.00	1.00	1.00	N.I.	N.I.	N.I.	0.01	0.50	0.50
155	DH-12	431.42	472.50	-294.03	-335.12	4.23	1.00	1.00	1.00	0.01	0.10	0.10	0.02	0.50	0.50
156	DH-12	388.90	429.68	-251.52	-292.29	3.78	0.50	1.00	1.00	0.20	0.05	0.01	0.02	0.50	0.50
157	DH-12	345.90	387.18	-208.52	-249.79	3.67	0.39	1.00	1.00	0.02	0.20	0.05	0.02	0.50	0.50
158	DH-12	279.40	344.67	-142.01	-207.29	4.07	1.00	1.00	1.00	0.02	0.01	0.03	0.01	0.50	0.50
153	DH-13	60.50	74.15	217.01	203.36	4.38	1.00	1.00	1.00	0.10	0.20	0.03	0.05	0.50	0.50
154	DH-13	408.00	442.05	-130.49	-164.54	3.44	0.05	1.00	1.00	0.05	0.20	0.12	0.02	0.50	0.50
160	MIU-4	82.29	116.45	134.70	100.54	4.25	1.00	1.00	1.00	0.00	0.20	0.03	0.02	0.50	0.50
161	MIU-4	272.75	274.49	-55.76	-57.50	4.03	0.38	1.00	1.00	0.05	0.20	0.00	0.40	0.50	0.50
162	MIU-4	505.76	560.41	-288.77	-343.42	3.72	0.38	1.00	1.00	0.10	0.20	0.03	0.01	0.50	0.50
163	MIU-4	653.42	684.25	-436.23	-422.26	4.10	0.71	0.93	1.00	0.20	0.20	0.03	0.02	0.50	0.50
166	MSB-2	171.49	175.49	27.00	23.00	3.86	0.44	1.00	1.00	0.20	0.02	0.02	0.18	0.50	0.50

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TOKI GRANITE															
167	MSB-4	95.50	99.00	118.95	115.45	4.21	1.00	0.85	1.00	0.10	0.05	0.01	0.20	0.50	0.50
N.G.	MIZ-1	113.05	116.28	N.R.	N.R.	4.35	1.00	1.00	1.00	0.10	0.02	0.02	0.22	0.50	0.50
N.G.	MIZ-1	215.00	225.67	N.R.	N.R.	2.89	0.34	0.42	1.00	0.01	0.05	0.00	0.07	0.50	0.50
TONO MINE (FORMATION, LITHOLOGY N.R.)															
57	gallery A+C	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
58	gallery B	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
59	gallery A+C	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
60	gallery B	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
61	20m S. gallery drop	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
62	30m S. gallery drop	N.R.	N.R.	N.R.	N.R.	1.09	N.I.	0.50	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
63	main gallery, 65 m boring	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
64	main gallery, 65 m boring	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
65	main gallery, 70 m boring	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TONO MINE (FORMATION, LITHOLOGY N.R.)															
66	main gallery, 70 m boring	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
67	main gallery, 95m boring	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
68	main gallery, 95m boring	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
69	main gallery, 120m boring	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
70	main gallery, 120m boring	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
71	north gallery, end	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
72	north gallery, end	N.R.	N.R.	N.R.	N.R.	1.37	N.I.	0.79	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
73	Under gallery, higashidobira boring	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
74	Under gallery, higashidobira boring	N.R.	N.R.	N.R.	N.R.	1.28	N.I.	0.70	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
75	Under gallery, ki eki drain	N.R.	N.R.	N.R.	N.R.	1.07	N.I.	0.48	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
TONO MINE (FORMATION, LITHOLOGY N.R.)															
76	Under gallery, cross cut #1W	N.R.	N.R.	N.R.	N.R.	1.39	N.I.	0.80	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
77	Under gallery, Tsukiyoshi f. drop	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
78	Under gallery, Tsukiyoshi f. pool	N.R.	N.R.	N.R.	N.R.	0.73	N.I.	0.14	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
99	T 08;Main drift 70m from No.1shaft	N.R.	N.R.	N.R.	N.R.	1.04	N.I.	0.46	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
100	T 09 (KNA 2)	N.R.	N.R.	N.R.	N.R.	1.09	N.I.	0.51	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
101	T 10;Main drift 120m from No.1 shaft	N.R.	N.R.	N.R.	N.R.	1.04	N.I.	0.46	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
102	T 11 (KS 1)	N.R.	N.R.	N.R.	N.R.	1.08	N.I.	0.50	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
103	T 12 (KNA 1)	N.R.	N.R.	N.R.	N.R.	1.20	N.I.	0.62	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
104	T 13 (Lower drift)	N.R.	N.R.	N.R.	N.R.	1.13	N.I.	0.54	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
OTHER BOREHOLES (FORMATION, LITHOLOGY N.R.)															
79	Matsunoke boring #1	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
80	Matsunoke boring #1	N.R.	N.R.	N.R.	N.R.	0.99	N.I.	0.41	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
81	Tsuk. Comm. Cntr. kimei81	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
82	Tsuk. Comm. Cntr. kimei81	N.R.	N.R.	N.R.	N.R.	0.71	N.I.	0.13	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
83	Kiguchi #81 boring	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
84	Kiguchi #81 boring	N.R.	N.R.	N.R.	N.R.	1.18	N.I.	0.60	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
ONSEN															
85	Oniiwa Onsen	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Komatsuya Onsen	N.R.	N.R.	N.R.	N.R.	1.58	N.I.	1.00	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Komatsuya Onsen	N.R.	N.R.	N.R.	N.R.	1.57	N.I.	0.99	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Takasago Onsen	701.10	1210.00	N.R.	N.R.	2.08	N.I.	1.00	0.25	N.I.	N.I.	N.I.	0.00	0.50	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
ONSEN															
N.G.	Takasago Onsen	701.10	1210.00	N.R.	N.R.	2.03	N.I.	0.94	0.25	N.I.	N.I.	N.I.	0.00	0.50	0.33
URANIUM EXPLORATION				*g.l. elevation											
N.G.	A 18	N.R.	N.R.	N.R.	N.R.	1.06	N.I.	0.48	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	A 18	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	A 73	N.R.	N.R.	N.R.	N.R.	1.05	N.I.	0.46	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	A 73'	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	E 17	N.R.	85.00	319.83	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	E 17	N.R.	85.00	319.83	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	E 18	N.R.	111.00	328.49	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 54	N.R.	101.00	132.64	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 55	N.R.	155.00	132.45	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 55	N.R.	155.00	132.45	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 58	N.R.	133.00	128.37	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 69	N.R.	317.00	157.75	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 69	N.R.	317.00	157.75	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
URANIUM EXPLORATION															
N.G.	G 81	N.R.	261.00	137.61	N.R.	1.08	N.I.	0.49	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 81	N.R.	261.00	137.61	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 87	N.R.	200.00	189.95	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	G 87	N.R.	200.00	189.95	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	IWA 25	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	K 2	N.R.	53.00	134.55	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 130	N.R.	72.00	262.54	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 165	N.R.	97.00	201.51	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 167	N.R.	64.00	199.22	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 182	N.R.	137.00	233.11	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 183	N.R.	131.00	229.15	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 183	N.R.	131.00	229.15	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 188	N.R.	153.00	170.72	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 188	N.R.	153.00	170.72	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 222	N.R.	190.00	158.52	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 222	N.R.	190.00	158.52	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

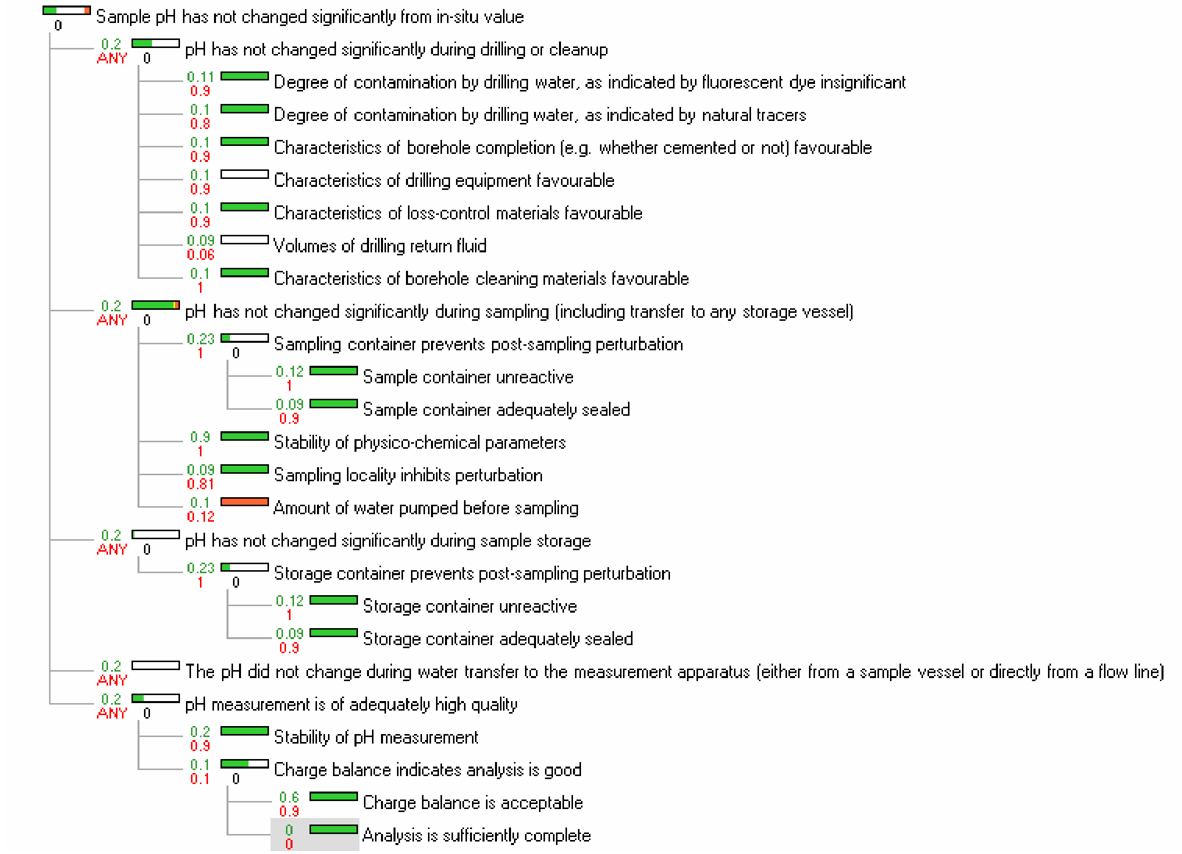
Table A1-1 continued.

Index	Location	Depth		Elevation		Scoring system									
							Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.	OVERALL QUALITY SCORE	Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
URANIUM EXPLORATION															
N.G.	MS 30	N.R.	148.00	167.35	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	MS 34	N.R.	219.00	158.22	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 114	N.R.	41.00	167.03	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 116	N.R.	172.00	147.04	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 116	N.R.	172.00	147.04	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 115	N.R.	149.00	145.50	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 115	N.R.	149.00	145.50	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 117	N.R.	42.00	146.11	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 119	N.R.	166.00	143.00	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 121	N.R.	96.00	142.82	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 121	N.R.	96.00	142.82	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 126	N.R.	38.00	147.67	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 126	N.R.	38.00	147.67	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 128	N.R.	109.00	141.65	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	S 128	N.R.	109.00	141.65	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Shizuhoragawa	N.R.	N.R.	N.R.	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

Table A1-1 continued.

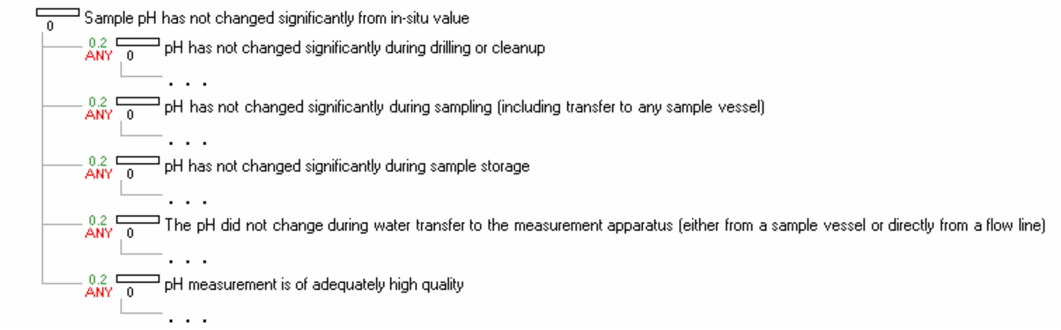
Index	Location	Depth		Elevation		Scoring system									
						OVERALL QUALITY SCORE	Scores corresponding to individual quality indicators								
		Min.	Max.	Min.	Max.		Drilling Fluid contamination	Charge balance	Lag time between sampling and analyses	pH stability	EC stability	Eh stability	Distance between packers	Sampling location	Physico-chemical parameter measuring location
		mbgl	mbgl	masl	masl		max=1	max=1	max=1	max=0.2	max=0.2	max=0.2	max=1	max=1	max=1
URANIUM EXPLORATION															
N.G.	TU 27	N.R.	150.00	224.31	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	TU 27	N.R.	150.00	224.31	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	TU 32	N.R.	112.00	232.57	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	TU 32	N.R.	112.00	232.57	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	TU 50	N.R.	91.00	302.64	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 13	N.R.	105.00	151.09	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 13	N.R.	105.00	151.09	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 3	N.R.	63.00	145.32	N.R.	0.79	N.I.	0.21	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 3	N.R.	63.00	145.32	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 40	N.R.	185.00	144.10	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 40	N.R.	185.00	144.10	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33
N.G.	Z 41	N.R.	195.00	159.73	N.R.	0.58	N.I.	N.I.	0.25	N.I.	N.I.	N.I.	N.I.	N.I.	0.33

Appendix 2 Draft process models

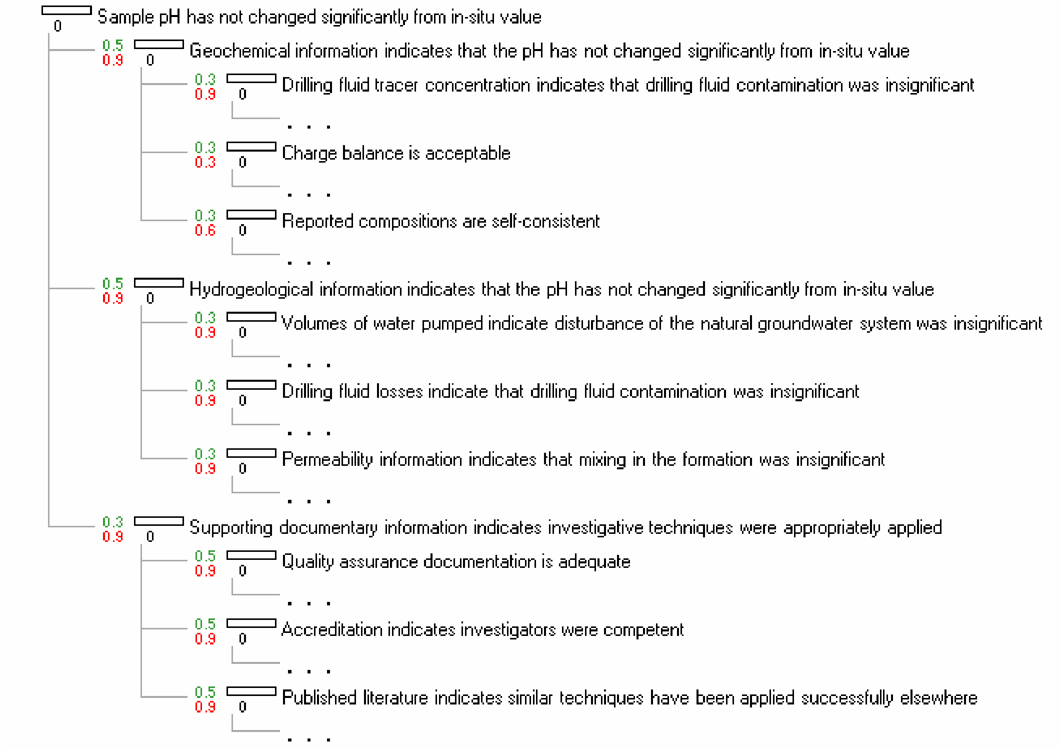


- 0 Sample pH has not changed significantly from in-situ value
  - 0.2 ANY 0 pH has not changed significantly during drilling or cleanup
    - 0.11 0.9 Degree of contamination by drilling water, as indicated by fluorescent dye insignificant
    - 0.1 0.8 Degree of contamination by drilling water, as indicated by natural tracers
    - 0.1 0.9 Characteristics of borehole completion (e.g. whether cemented or not) favourable
    - 0.1 0.9 Characteristics of drilling equipment favourable
    - 0.1 0.9 Characteristics of loss-control materials favourable
    - 0.09 0.06 Volumes of drilling return fluid
    - 0.1 1 Characteristics of borehole cleaning materials favourable
  - 0.2 ANY 0 pH has not changed significantly during sampling (including transfer to any storage vessel)
    - 0.23 1 0 Sampling container prevents post-sampling perturbation
      - 0.12 1 Sample container unreactive
      - 0.09 0.9 Sample container adequately sealed
    - 0.9 1 Stability of physico-chemical parameters
    - 0.09 0.81 Sampling locality inhibits perturbation
    - 0.1 0.12 Amount of water pumped before sampling
  - 0.2 ANY 0 pH has not changed significantly during sample storage
    - 0.23 1 0 Storage container prevents post-sampling perturbation
      - 0.12 1 Storage container unreactive
      - 0.09 0.9 Storage container adequately sealed
  - 0.2 ANY The pH did not change during water transfer to the measurement apparatus (either from a sample vessel or directly from a flow line)
  - 0.2 ANY 0 pH measurement is of adequately high quality
    - 0.2 0.9 Stability of pH measurement
    - 0.1 0.1 0 Charge balance indicates analysis is good
      - 0.6 0.9 Charge balance is acceptable
      - 0 0 Analysis is sufficiently complete

Summary overall draft process model.

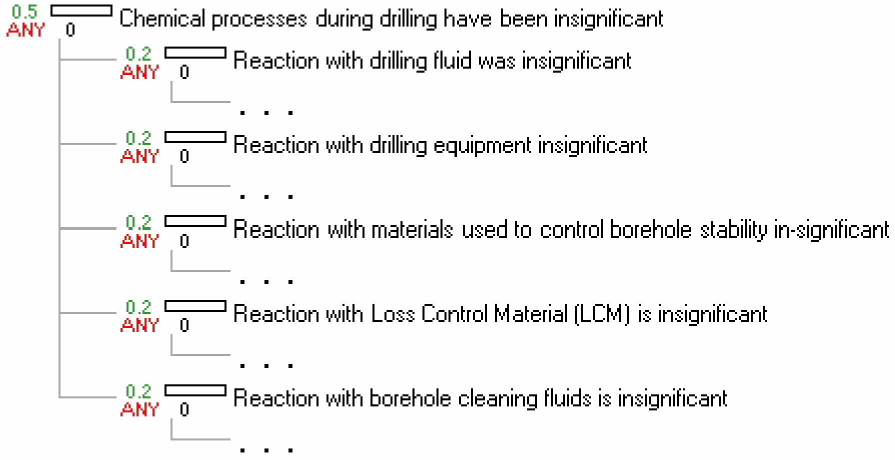


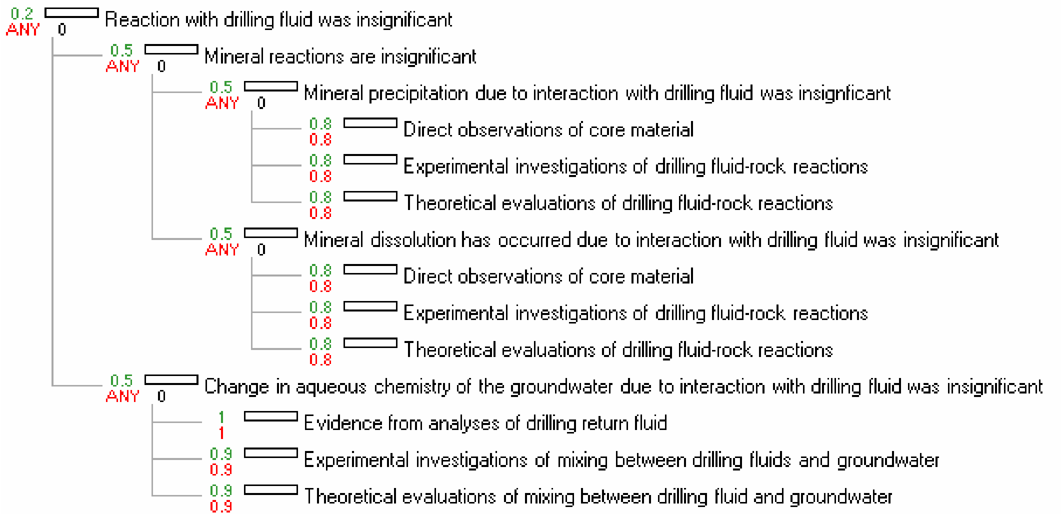
- 0 Sample pH has not changed significantly from in-situ value
  - 0.2 ANY 0 pH has not changed significantly during drilling or cleanup
    - . . .
  - 0.2 ANY 0 pH has not changed significantly during sampling (including transfer to any sample vessel)
    - . . .
  - 0.2 ANY 0 pH has not changed significantly during sample storage
    - . . .
  - 0.2 ANY 0 The pH did not change during water transfer to the measurement apparatus (either from a sample vessel or directly from a flow line)
    - . . .
  - 0.2 ANY 0 pH measurement is of adequately high quality
    - . . .

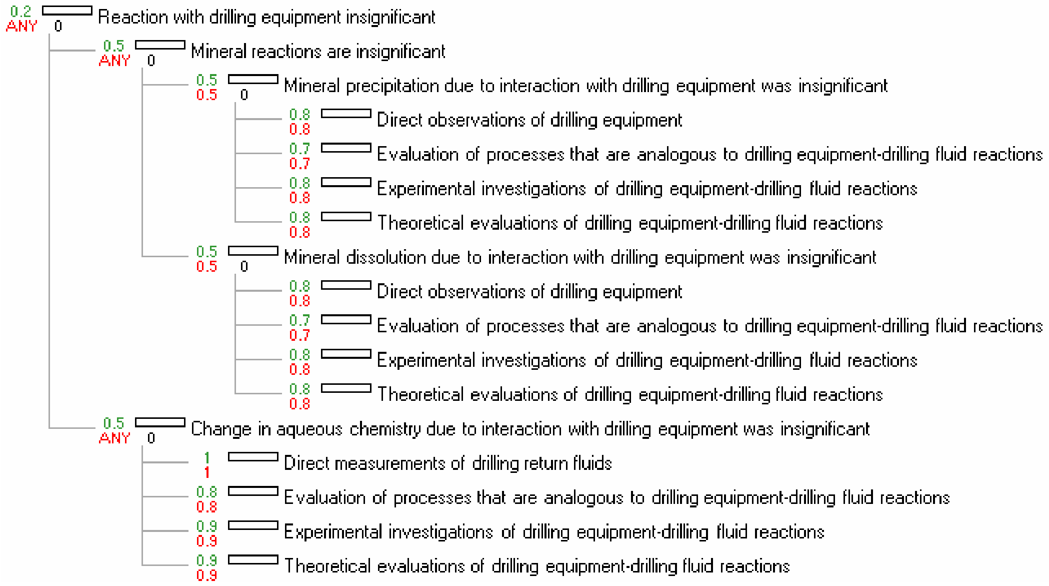


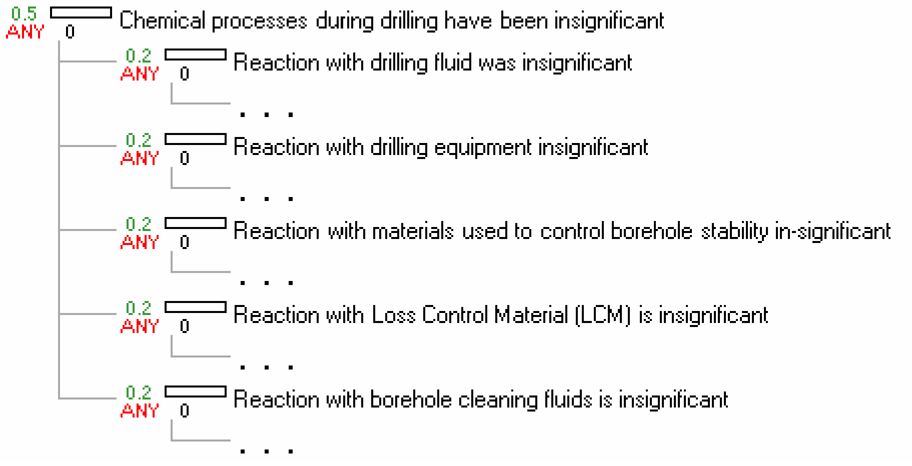
- 0 Sample pH has not changed significantly from in-situ value
  - 0.5 0.9 0 Geochemical information indicates that the pH has not changed significantly from in-situ value
    - 0.3 0.9 0 Drilling fluid tracer concentration indicates that drilling fluid contamination was insignificant
      - . . .
    - 0.3 0.3 0 Charge balance is acceptable
      - . . .
    - 0.3 0.6 0 Reported compositions are self-consistent
      - . . .
  - 0.5 0.9 0 Hydrogeological information indicates that the pH has not changed significantly from in-situ value
    - 0.3 0.9 0 Volumes of water pumped indicate disturbance of the natural groundwater system was insignificant
      - . . .
    - 0.3 0.9 0 Drilling fluid losses indicate that drilling fluid contamination was insignificant
      - . . .
    - 0.3 0.9 0 Permeability information indicates that mixing in the formation was insignificant
      - . . .
  - 0.3 0.9 0 Supporting documentary information indicates investigative techniques were appropriately applied
    - 0.5 0.9 0 Quality assurance documentation is adequate
      - . . .
    - 0.5 0.9 0 Accreditation indicates investigators were competent
      - . . .
    - 0.5 0.9 0 Published literature indicates similar techniques have been applied successfully elsewhere
      - . . .

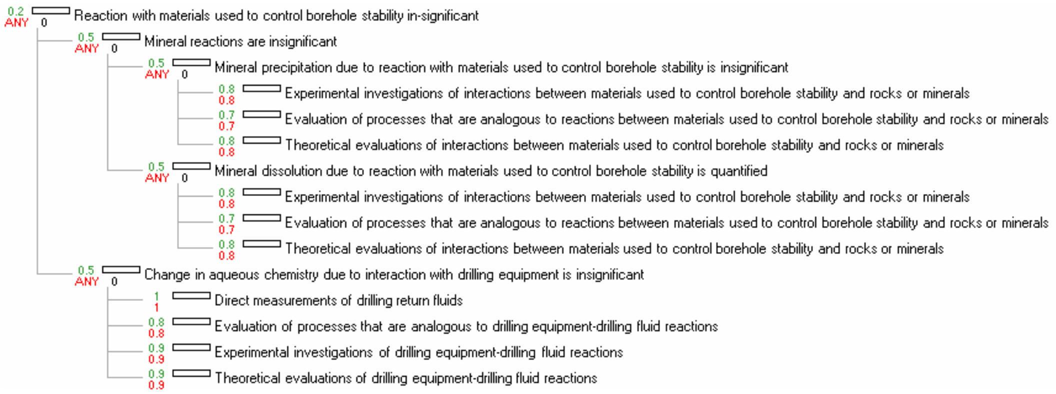

0 Sample pH has not changed significantly from in-situ value
0.2 ANY 0 pH has not changed significantly during drilling or cleanup
0.5 ANY 0 Chemical processes during drilling have been insignificant
. . .
0.5 ANY 0 Physical processes during drilling have been insignificant
. . .
0.2 ANY 0 pH has not changed significantly during sampling (including transfer to any sample vessel)
1 1 0 Observations in the evaluated borehole indicate that pH did not change significantly during sampling (including transfer to any sample vessel)
1 1 0 Observations in the evaluated test section indicate that pH did not change significantly during sampling (including transfer to any sample vessel)
0.5 ANY 0 Observations in the evaluated test section indicate that chemical processes during sampling were insignificant
. . .
0.5 ANY 0 Observations in the evaluated test section indicate that physical processes during sampling were insignificant
. . .
0.9 ANY Stability of flow-through cell measurements
0.7 0.9 0 Observations in other test sections in the evaluated borehole indicate that pH did not change significantly during sampling (including transfer to any sample vessel)
0.5 ANY 0 Observations in other test sections in the evaluated borehole indicate that chemical processes during sampling were insignificant
. . .
0.5 ANY 0 Observations in other test sections in the evaluated borehole indicate that physical processes during sampling were insignificant
. . .
0.7 0.9 0 Observations in other boreholes indicate that pH did not change significantly during sampling (including transfer to any sample vessel)
0.5 ANY 0 Chemical processes during sampling from other boreholes were insignificant
. . .
0.5 ANY 0 Physical processes during sampling from other boreholes were insignificant
. . .
0.2 ANY 0 pH has not changed significantly during sample storage
1 0 The sample was not stored before measurement
1 1 0 Chemical and physical processes did not change the pH significantly during storage
0.5 ANY 0 Chemical processes during storage were insignificant
. . .
0.5 ANY 0 Physical processes during storage were insignificant
. . .
0.2 ANY 0 The pH did not change during water transfer to the measurement apparatus (either from a sample vessel or directly from a flow line)
1 0 The measurement of pH did not involve transfer from the sampling apparatus
1 1 0 Chemical and physical processes did not change the pH significantly during transfer
0.5 ANY 0 Chemical processes during transfer were insignificant
. . .
0.5 ANY 0 Physical processes during transfer were insignificant
. . .
0.2 ANY 0 pH measurement is of adequately high quality
1 1 0 Characteristics of measurements indicate pH measurements were adequate
. . .
0.8 0.8 0 Literature information indicates pH measurements were adequate
. . .


0.5 ANY 0 Chemical processes during drilling have been insignificant
0.2 ANY 0 Reaction with drilling fluid was insignificant
. . .
0.2 ANY 0 Reaction with drilling equipment insignificant
. . .
0.2 ANY 0 Reaction with materials used to control borehole stability in-significant
. . .
0.2 ANY 0 Reaction with Loss Control Material (LCM) is insignificant
. . .
0.2 ANY 0 Reaction with borehole cleaning fluids is insignificant
. . .

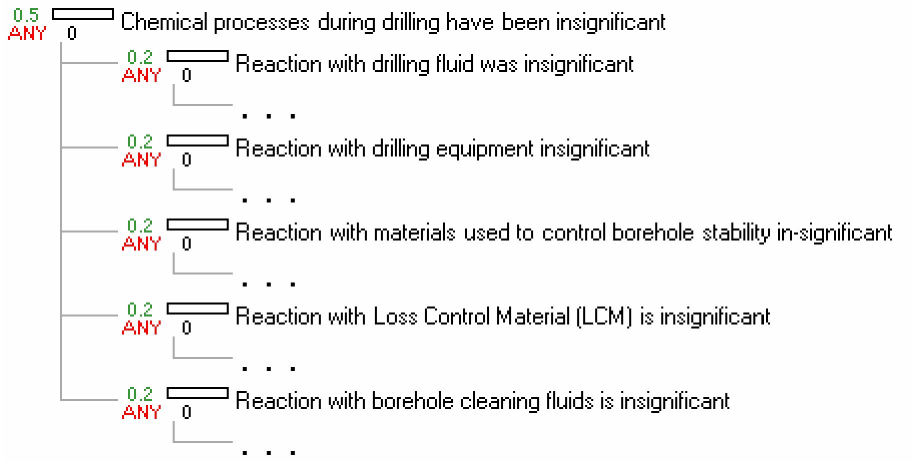

0.2 ANY 0 Reaction with drilling fluid was insignificant
0.5 ANY 0 Mineral reactions are insignificant
0.5 ANY 0 Mineral precipitation due to interaction with drilling fluid was insignficant
0.8 0.8 Direct observations of core material
0.8 0.8 Experimental investigations of drilling fluid-rock reactions
0.8 0.8 Theoretical evaluations of drilling fluid-rock reactions
0.5 ANY 0 Mineral dissolution has occurred due to interaction with drilling fluid was insignificant
0.8 0.8 Direct observations of core material
0.8 0.8 Experimental investigations of drilling fluid-rock reactions
0.8 0.8 Theoretical evaluations of drilling fluid-rock reactions
0.5 ANY 0 Change in aqueous chemistry of the groundwater due to interaction with drilling fluid was insignificant
1 1 Evidence from analyses of drilling return fluid
0.9 0.9 Experimental investigations of mixing between drilling fluids and groundwater
0.9 0.9 Theoretical evaluations of mixing between drilling fluid and groundwater


0.2 ANY 0 Reaction with drilling equipment insignificant
0.5 ANY 0 Mineral reactions are insignificant
0.5 0.5 0 Mineral precipitation due to interaction with drilling equipment was insignificant
0.8 0.8 Direct observations of drilling equipment
0.7 0.7 Evaluation of processes that are analogous to drilling equipment-drilling fluid reactions
0.8 0.8 Experimental investigations of drilling equipment-drilling fluid reactions
0.8 0.8 Theoretical evaluations of drilling equipment-drilling fluid reactions
0.5 0.5 0 Mineral dissolution due to interaction with drilling equipment was insignificant
0.8 0.8 Direct observations of drilling equipment
0.7 0.7 Evaluation of processes that are analogous to drilling equipment-drilling fluid reactions
0.8 0.8 Experimental investigations of drilling equipment-drilling fluid reactions
0.8 0.8 Theoretical evaluations of drilling equipment-drilling fluid reactions
0.5 ANY 0 Change in aqueous chemistry due to interaction with drilling equipment was insignificant
1 1 Direct measurements of drilling return fluids
0.8 0.8 Evaluation of processes that are analogous to drilling equipment-drilling fluid reactions
0.9 0.9 Experimental investigations of drilling equipment-drilling fluid reactions
0.9 0.9 Theoretical evaluations of drilling equipment-drilling fluid reactions

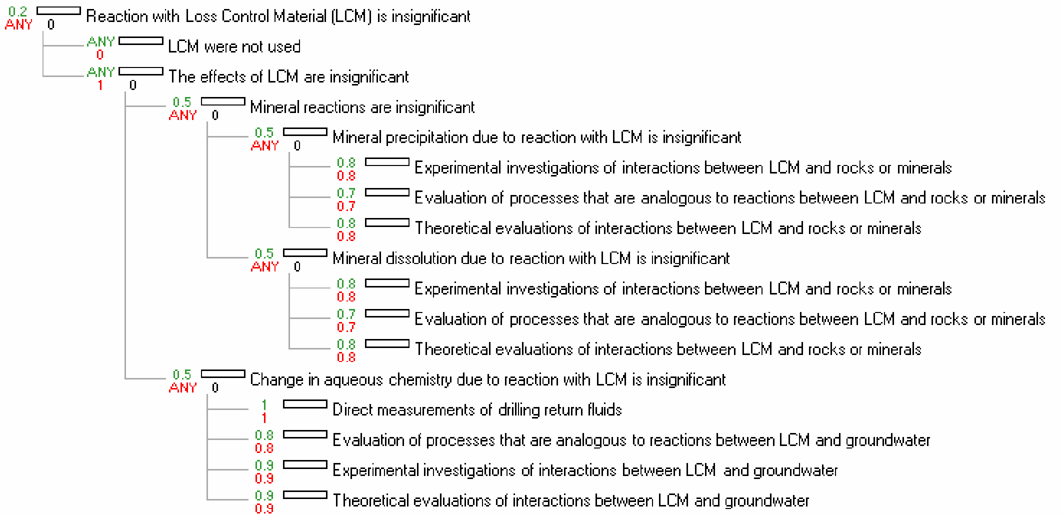

0.5 ANY 0 Chemical processes during drilling have been insignificant
0.2 ANY 0 Reaction with drilling fluid was insignificant
. . .
0.2 ANY 0 Reaction with drilling equipment insignificant
. . .
0.2 ANY 0 Reaction with materials used to control borehole stability in-significant
. . .
0.2 ANY 0 Reaction with Loss Control Material (LCM) is insignificant
. . .
0.2 ANY 0 Reaction with borehole cleaning fluids is insignificant
. . .



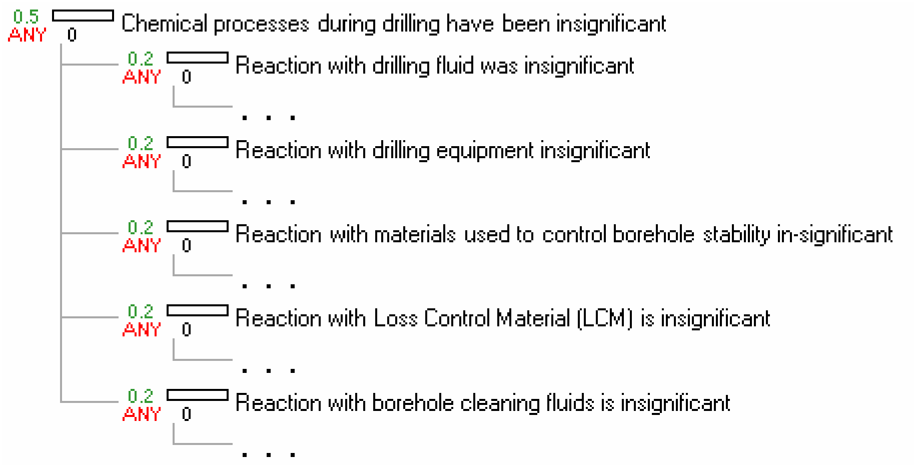
- 0.2 ANY 0 Reaction with materials used to control borehole stability in-significant
  - 0.5 ANY 0 Mineral reactions are insignificant
    - 0.5 ANY 0 Mineral precipitation due to reaction with materials used to control borehole stability is insignificant
      - 0.8 0.8 Experimental investigations of interactions between materials used to control borehole stability and rocks or minerals
      - 0.7 0.7 Evaluation of processes that are analogous to reactions between materials used to control borehole stability and rocks or minerals
      - 0.8 0.8 Theoretical evaluations of interactions between materials used to control borehole stability and rocks or minerals
    - 0.5 ANY 0 Mineral dissolution due to reaction with materials used to control borehole stability is quantified
      - 0.8 0.8 Experimental investigations of interactions between materials used to control borehole stability and rocks or minerals
      - 0.7 0.7 Evaluation of processes that are analogous to reactions between materials used to control borehole stability and rocks or minerals
      - 0.8 0.8 Theoretical evaluations of interactions between materials used to control borehole stability and rocks or minerals
  - 0.5 ANY 0 Change in aqueous chemistry due to interaction with drilling equipment is insignificant
    - 1 1 Direct measurements of drilling return fluids
    - 0.8 0.8 Evaluation of processes that are analogous to drilling equipment-drilling fluid reactions
    - 0.9 0.9 Experimental investigations of drilling equipment-drilling fluid reactions
    - 0.9 0.9 Theoretical evaluations of drilling equipment-drilling fluid reactions

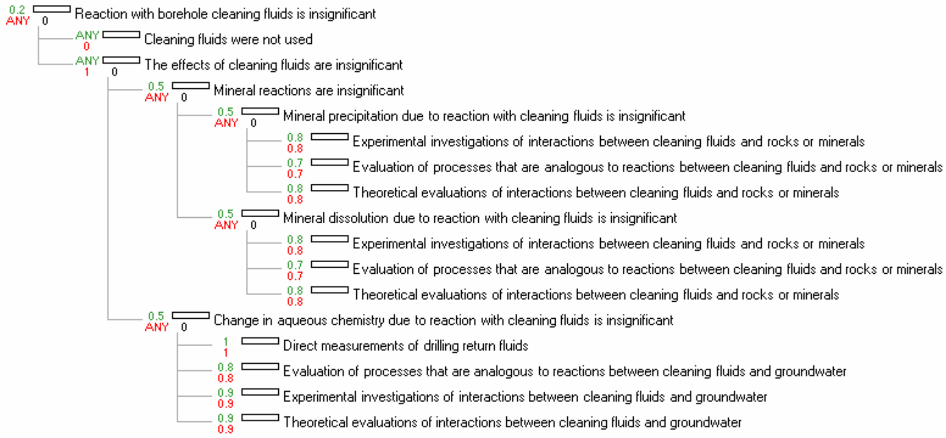


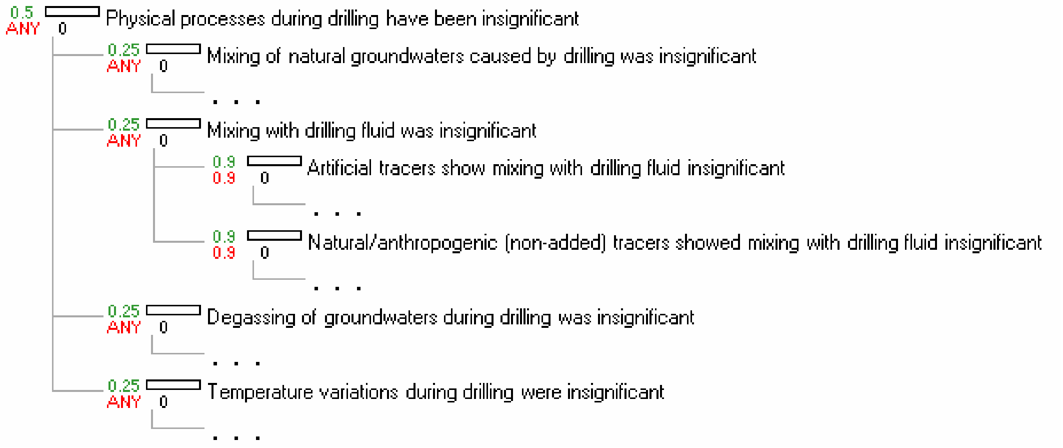
- 0.5 ANY 0 Chemical processes during drilling have been insignificant
  - 0.2 ANY 0 Reaction with drilling fluid was insignificant
    - . . .
  - 0.2 ANY 0 Reaction with drilling equipment insignificant
    - . . .
  - 0.2 ANY 0 Reaction with materials used to control borehole stability in-significant
    - . . .
  - 0.2 ANY 0 Reaction with Loss Control Material (LCM) is insignificant
    - . . .
  - 0.2 ANY 0 Reaction with borehole cleaning fluids is insignificant
    - . . .

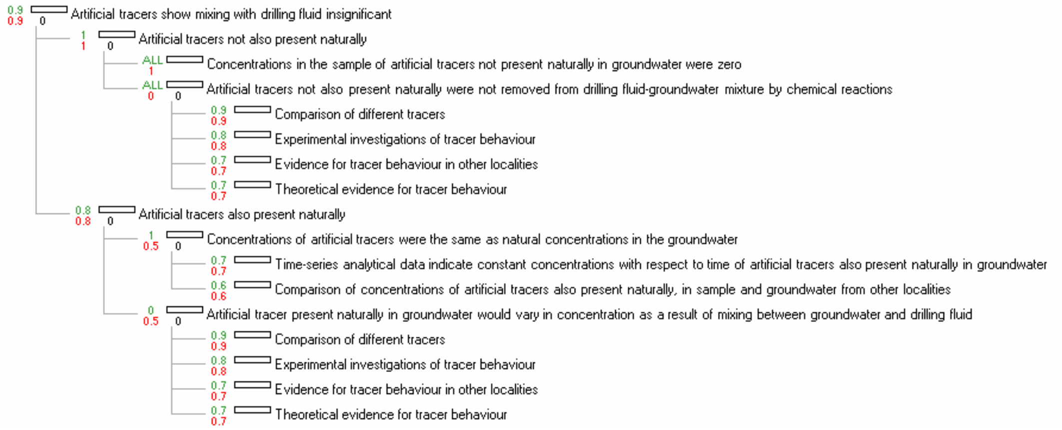


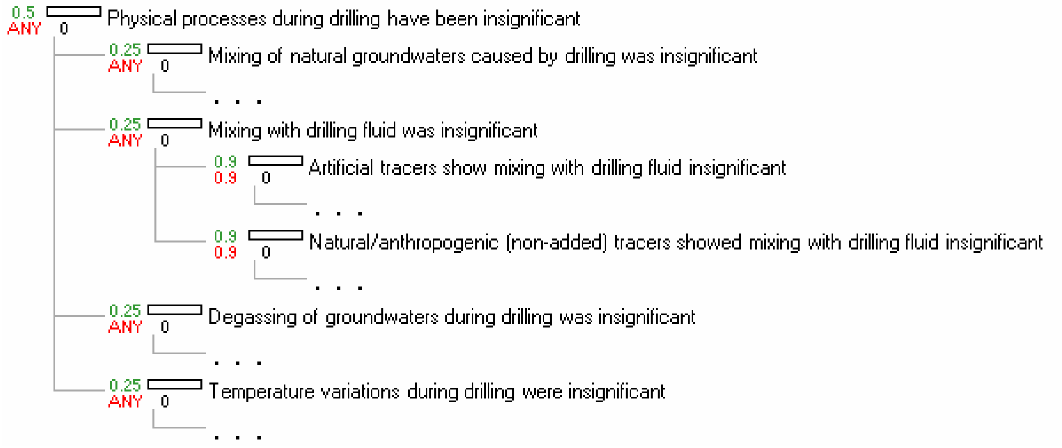
- 0.2 ANY 0 Reaction with Loss Control Material (LCM) is insignificant
  - ANY 0 LCM were not used
  - ANY 1 0 The effects of LCM are insignificant
    - 0.5 ANY 0 Mineral reactions are insignificant
      - 0.5 ANY 0 Mineral precipitation due to reaction with LCM is insignificant
        - 0.8 0.8 Experimental investigations of interactions between LCM and rocks or minerals
        - 0.7 0.7 Evaluation of processes that are analogous to reactions between LCM and rocks or minerals
        - 0.8 0.8 Theoretical evaluations of interactions between LCM and rocks or minerals
      - 0.5 ANY 0 Mineral dissolution due to reaction with LCM is insignificant
        - 0.8 0.8 Experimental investigations of interactions between LCM and rocks or minerals
        - 0.7 0.7 Evaluation of processes that are analogous to reactions between LCM and rocks or minerals
        - 0.8 0.8 Theoretical evaluations of interactions between LCM and rocks or minerals
    - 0.5 ANY 0 Change in aqueous chemistry due to reaction with LCM is insignificant
      - 1 1 Direct measurements of drilling return fluids
      - 0.8 0.8 Evaluation of processes that are analogous to reactions between LCM and groundwater
      - 0.9 0.9 Experimental investigations of interactions between LCM and groundwater
      - 0.9 0.9 Theoretical evaluations of interactions between LCM and groundwater

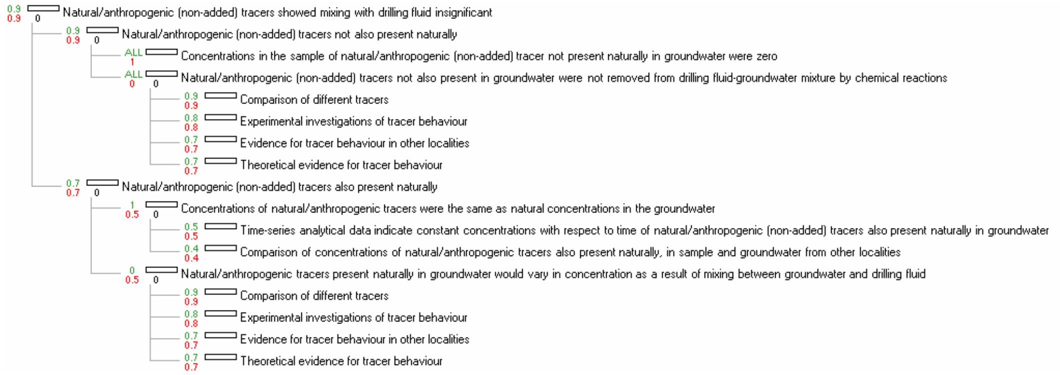

0.5 ANY 0 Chemical processes during drilling have been insignificant
0.2 ANY 0 Reaction with drilling fluid was insignificant
. . .
0.2 ANY 0 Reaction with drilling equipment insignificant
. . .
0.2 ANY 0 Reaction with materials used to control borehole stability in-significant
. . .
0.2 ANY 0 Reaction with Loss Control Material (LCM) is insignificant
. . .
0.2 ANY 0 Reaction with borehole cleaning fluids is insignificant
. . .

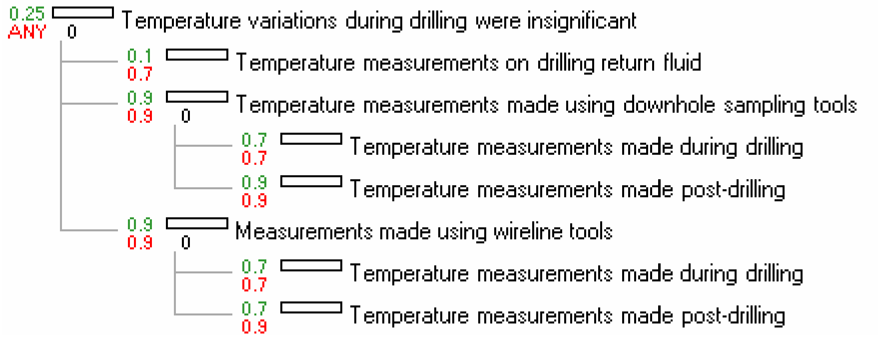

0.2 ANY 0 Reaction with borehole cleaning fluids is insignificant
ANY 0 Cleaning fluids were not used
ANY 1 0 The effects of cleaning fluids are insignificant
0.5 ANY 0 Mineral reactions are insignificant
0.5 ANY 0 Mineral precipitation due to reaction with cleaning fluids is insignificant
0.8 0.8 Experimental investigations of interactions between cleaning fluids and rocks or minerals
0.7 0.7 Evaluation of processes that are analogous to reactions between cleaning fluids and rocks or minerals
0.8 0.8 Theoretical evaluations of interactions between cleaning fluids and rocks or minerals
0.5 ANY 0 Mineral dissolution due to reaction with cleaning fluids is insignificant
0.8 0.8 Experimental investigations of interactions between cleaning fluids and rocks or minerals
0.7 0.7 Evaluation of processes that are analogous to reactions between cleaning fluids and rocks or minerals
0.8 0.8 Theoretical evaluations of interactions between cleaning fluids and rocks or minerals
0.5 ANY 0 Change in aqueous chemistry due to reaction with cleaning fluids is insignificant
1 1 Direct measurements of drilling return fluids
0.8 0.8 Evaluation of processes that are analogous to reactions between cleaning fluids and groundwater
0.9 0.9 Experimental investigations of interactions between cleaning fluids and groundwater
0.9 0.9 Theoretical evaluations of interactions between cleaning fluids and groundwater


0.5 ANY 0 Physical processes during drilling have been insignificant
0.25 ANY 0 Mixing of natural groundwaters caused by drilling was insignificant
. . .
0.25 ANY 0 Mixing with drilling fluid was insignificant
0.9 0.9 0 Artificial tracers show mixing with drilling fluid insignificant
. . .
0.9 0.9 0 Natural/anthropogenic (non-added) tracers showed mixing with drilling fluid insignificant
. . .
0.25 ANY 0 Degassing of groundwaters during drilling was insignificant
. . .
0.25 ANY 0 Temperature variations during drilling were insignificant
. . .

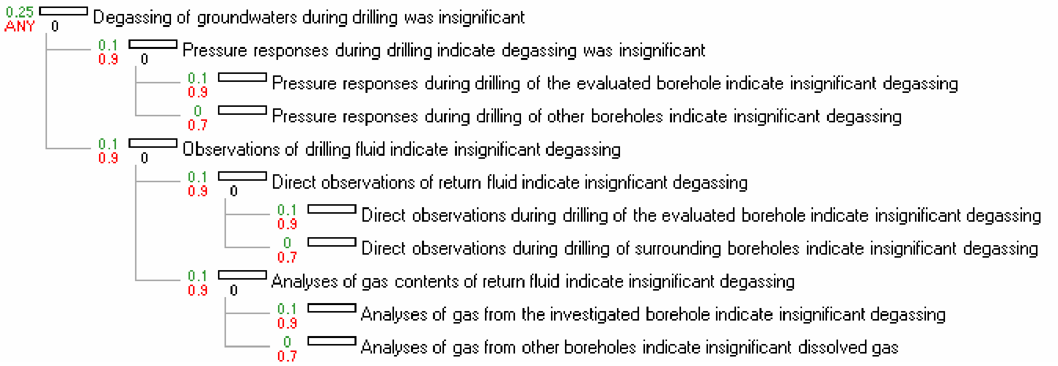

0.9 0.9 0 Artificial tracers show mixing with drilling fluid insignificant
1 1 0 Artificial tracers not also present naturally
ALL 1 Concentrations in the sample of artificial tracers not present naturally in groundwater were zero
ALL 0 0 Artificial tracers not also present naturally were not removed from drilling fluid-groundwater mixture by chemical reactions
0.9 0.9 Comparison of different tracers
0.8 0.8 Experimental investigations of tracer behaviour
0.7 0.7 Evidence for tracer behaviour in other localities
0.7 0.7 Theoretical evidence for tracer behaviour
0.8 0.8 0 Artificial tracers also present naturally
1 0.5 0 Concentrations of artificial tracers were the same as natural concentrations in the groundwater
0.7 0.7 Time-series analytical data indicate constant concentrations with respect to time of artificial tracers also present naturally in groundwater
0.6 0.6 Comparison of concentrations of artificial tracers also present naturally, in sample and groundwater from other localities
0 0.5 0 Artificial tracer present naturally in groundwater would vary in concentration as a result of mixing between groundwater and drilling fluid
0.9 0.9 Comparison of different tracers
0.8 0.8 Experimental investigations of tracer behaviour
0.7 0.7 Evidence for tracer behaviour in other localities
0.7 0.7 Theoretical evidence for tracer behaviour


0.5 ANY 0 Physical processes during drilling have been insignificant
0.25 ANY 0 Mixing of natural groundwaters caused by drilling was insignificant
. . .
0.25 ANY 0 Mixing with drilling fluid was insignificant
0.9 0.9 0 Artificial tracers show mixing with drilling fluid insignificant
. . .
0.9 0.9 0 Natural/anthropogenic (non-added) tracers showed mixing with drilling fluid insignificant
. . .
0.25 ANY 0 Degassing of groundwaters during drilling was insignificant
. . .
0.25 ANY 0 Temperature variations during drilling were insignificant
. . .

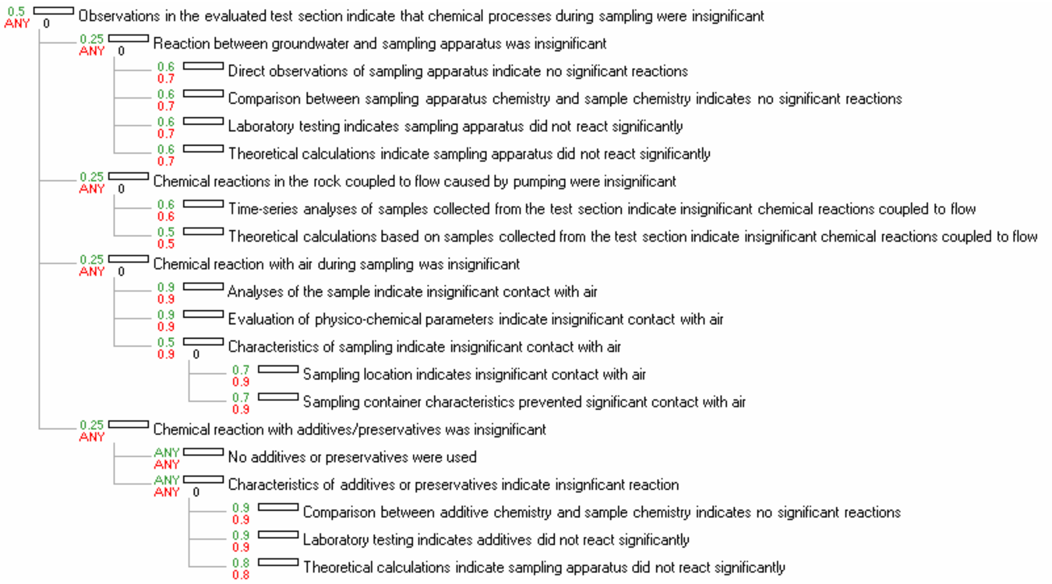

0.9 0.9 0 Natural/anthropogenic (non-added) tracers showed mixing with drilling fluid insignificant
0.9 0.9 0 Natural/anthropogenic (non-added) tracers not also present naturally
ALL 1 Concentrations in the sample of natural/anthropogenic (non-added) tracer not present naturally in groundwater were zero
ALL 0 0 Natural/anthropogenic (non-added) tracers not also present in groundwater were not removed from drilling fluid-groundwater mixture by chemical reactions
0.9 0.9 Comparison of different tracers
0.8 0.8 Experimental investigations of tracer behaviour
0.7 0.7 Evidence for tracer behaviour in other localities
0.7 0.7 Theoretical evidence for tracer behaviour
0.7 0.7 0 Natural/anthropogenic (non-added) tracers also present naturally
1 0.5 0 Concentrations of natural/anthropogenic tracers were the same as natural concentrations in the groundwater
0.5 0.5 Time-series analytical data indicate constant concentrations with respect to time of natural/anthropogenic (non-added) tracers also present naturally in groundwater
0.4 0.4 Comparison of concentrations of natural/anthropogenic tracers also present naturally, in sample and groundwater from other localities
0 0.5 0 Natural/anthropogenic tracers present naturally in groundwater would vary in concentration as a result of mixing between groundwater and drilling fluid
0.9 0.9 Comparison of different tracers
0.8 0.8 Experimental investigations of tracer behaviour
0.7 0.7 Evidence for tracer behaviour in other localities
0.7 0.7 Theoretical evidence for tracer behaviour



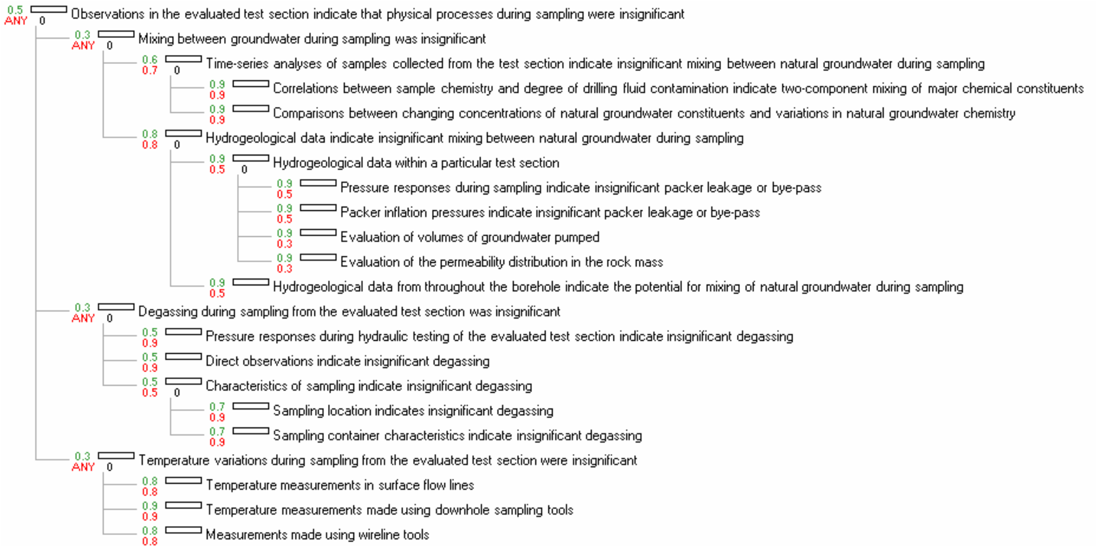
- 0.25 ANY 0 Temperature variations during drilling were insignificant
  - 0.1 0.7 Temperature measurements on drilling return fluid
  - 0.9 0.9 0 Temperature measurements made using downhole sampling tools
    - 0.7 0.7 Temperature measurements made during drilling
    - 0.9 0.9 Temperature measurements made post-drilling
  - 0.9 0.9 0 Measurements made using wireline tools
    - 0.7 0.7 Temperature measurements made during drilling
    - 0.7 0.9 Temperature measurements made post-drilling



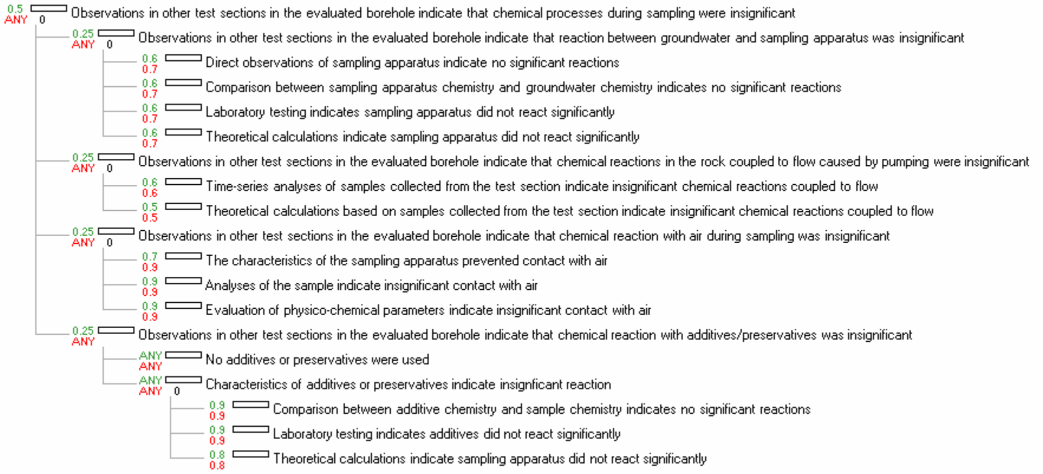
- 0.25 ANY 0 Degassing of groundwaters during drilling was insignificant
  - 0.1 0.9 0 Pressure responses during drilling indicate degassing was insignificant
    - 0.1 0.9 Pressure responses during drilling of the evaluated borehole indicate insignificant degassing
    - 0 0.7 Pressure responses during drilling of other boreholes indicate insignificant degassing
  - 0.1 0.9 0 Observations of drilling fluid indicate insignificant degassing
    - 0.1 0.9 0 Direct observations of return fluid indicate insignficant degassing
      - 0.1 0.9 Direct observations during drilling of the evaluated borehole indicate insignificant degassing
      - 0 0.7 Direct observations during drilling of surrounding boreholes indicate insignificant degassing
    - 0.1 0.9 0 Analyses of gas contents of return fluid indicate insignificant degassing
      - 0.1 0.9 Analyses of gas from the investigated borehole indicate insignificant degassing
      - 0 0.7 Analyses of gas from other boreholes indicate insignificant dissolved gas



- 0.5 ANY 0 Observations in the evaluated test section indicate that chemical processes during sampling were insignificant
  - 0.25 ANY 0 Reaction between groundwater and sampling apparatus was insignificant
    - 0.6 0.7 Direct observations of sampling apparatus indicate no significant reactions
    - 0.6 0.7 Comparison between sampling apparatus chemistry and sample chemistry indicates no significant reactions
    - 0.6 0.7 Laboratory testing indicates sampling apparatus did not react significantly
    - 0.6 0.7 Theoretical calculations indicate sampling apparatus did not react significantly
  - 0.25 ANY 0 Chemical reactions in the rock coupled to flow caused by pumping were insignificant
    - 0.6 0.6 Time-series analyses of samples collected from the test section indicate insignificant chemical reactions coupled to flow
    - 0.5 0.5 Theoretical calculations based on samples collected from the test section indicate insignificant chemical reactions coupled to flow
  - 0.25 ANY 0 Chemical reaction with air during sampling was insignificant
    - 0.9 0.9 Analyses of the sample indicate insignificant contact with air
    - 0.9 0.9 Evaluation of physico-chemical parameters indicate insignificant contact with air
    - 0.5 0.9 0 Characteristics of sampling indicate insignificant contact with air
      - 0.7 0.9 Sampling location indicates insignificant contact with air
      - 0.7 0.9 Sampling container characteristics prevented significant contact with air
  - 0.25 ANY Chemical reaction with additives/preservatives was insignificant
    - ANY ANY No additives or preservatives were used
    - ANY ANY 0 Characteristics of additives or preservatives indicate insignficant reaction
      - 0.9 0.9 Comparison between additive chemistry and sample chemistry indicates no significant reactions
      - 0.9 0.9 Laboratory testing indicates additives did not react significantly
      - 0.8 0.8 Theoretical calculations indicate sampling apparatus did not react significantly



- 0.5 ANY 0 Observations in the evaluated test section indicate that physical processes during sampling were insignificant
  - 0.3 ANY 0 Mixing between groundwater during sampling was insignificant
    - 0.6 0.7 0 Time-series analyses of samples collected from the test section indicate insignificant mixing between natural groundwater during sampling
      - 0.9 0.9 Correlations between sample chemistry and degree of drilling fluid contamination indicate two-component mixing of major chemical constituents
      - 0.9 0.9 Comparisons between changing concentrations of natural groundwater constituents and variations in natural groundwater chemistry
    - 0.8 0.8 0 Hydrogeological data indicate insignificant mixing between natural groundwater during sampling
      - 0.9 0.5 0 Hydrogeological data within a particular test section
        - 0.9 0.5 Pressure responses during sampling indicate insignificant packer leakage or bye-pass
        - 0.9 0.5 Packer inflation pressures indicate insignificant packer leakage or bye-pass
        - 0.9 0.3 Evaluation of volumes of groundwater pumped
        - 0.9 0.3 Evaluation of the permeability distribution in the rock mass
      - 0.9 0.5 Hydrogeological data from throughout the borehole indicate the potential for mixing of natural groundwater during sampling
  - 0.3 ANY 0 Degassing during sampling from the evaluated test section was insignificant
    - 0.5 0.9 Pressure responses during hydraulic testing of the evaluated test section indicate insignificant degassing
    - 0.5 0.9 Direct observations indicate insignificant degassing
    - 0.5 0.5 0 Characteristics of sampling indicate insignificant degassing
      - 0.7 0.9 Sampling location indicates insignificant degassing
      - 0.7 0.9 Sampling container characteristics indicate insignificant degassing
  - 0.3 ANY 0 Temperature variations during sampling from the evaluated test section were insignificant
    - 0.8 0.8 Temperature measurements in surface flow lines
    - 0.9 0.9 Temperature measurements made using downhole sampling tools
    - 0.8 0.8 Measurements made using wireline tools



- 0.5 ANY 0 Observations in other test sections in the evaluated borehole indicate that chemical processes during sampling were insignificant
  - 0.25 ANY 0 Observations in other test sections in the evaluated borehole indicate that reaction between groundwater and sampling apparatus was insignificant
    - 0.6 0.7 Direct observations of sampling apparatus indicate no significant reactions
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    - 0.6 0.7 Theoretical calculations indicate sampling apparatus did not react significantly
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    - 0.6 0.6 Time-series analyses of samples collected from the test section indicate insignificant chemical reactions coupled to flow
    - 0.5 0.5 Theoretical calculations based on samples collected from the test section indicate insignificant chemical reactions coupled to flow
  - 0.25 ANY 0 Observations in other test sections in the evaluated borehole indicate that chemical reaction with air during sampling was insignificant
    - 0.7 0.9 The characteristics of the sampling apparatus prevented contact with air
    - 0.9 0.9 Analyses of the sample indicate insignificant contact with air
    - 0.9 0.9 Evaluation of physico-chemical parameters indicate insignificant contact with air
  - 0.25 ANY Observations in other test sections in the evaluated borehole indicate that chemical reaction with additives/preservatives was insignificant
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    - ANY ANY 0 Characteristics of additives or preservatives indicate insignficant reaction
      - 0.9 0.9 Comparison between additive chemistry and sample chemistry indicates no significant reactions
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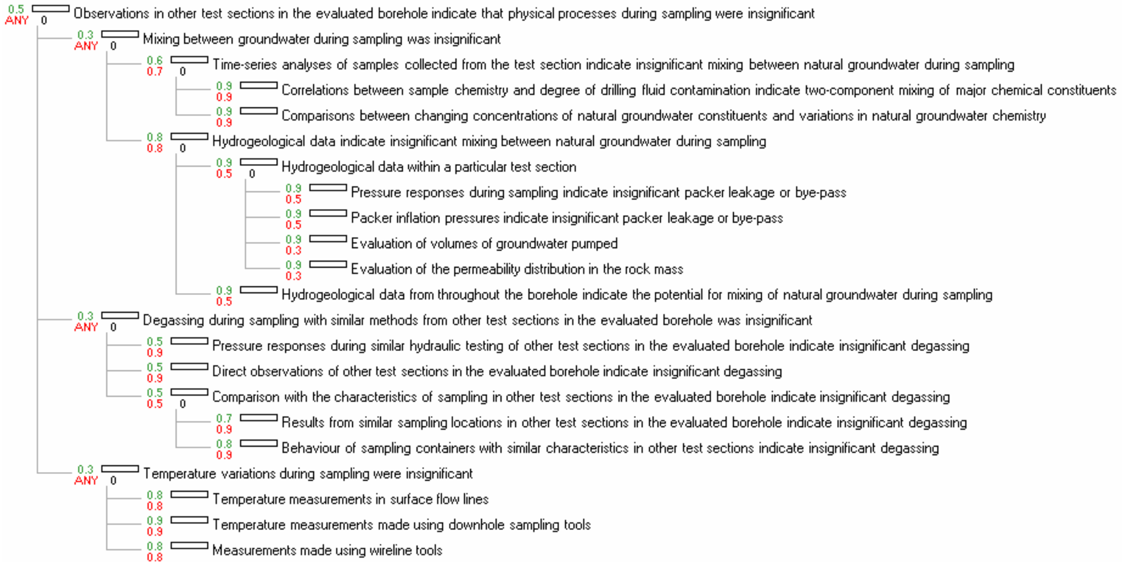
      - 0.8 0.8 Theoretical calculations indicate sampling apparatus did not react significantly



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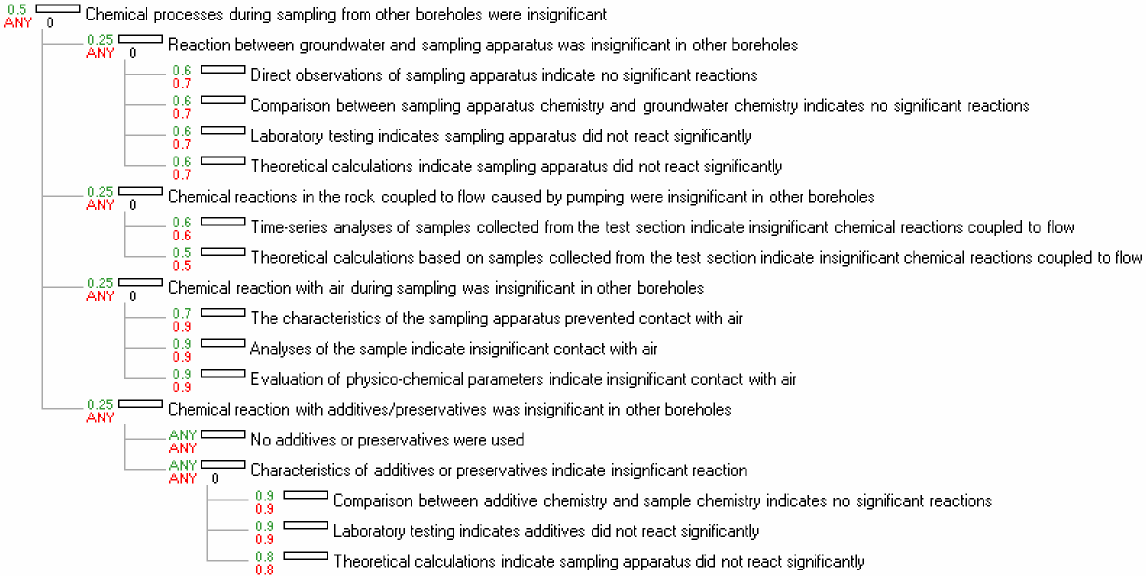
      - 0.9 0.5 Hydrogeological data from throughout the borehole indicate the potential for mixing of natural groundwater during sampling
  - 0.3 ANY 0 Degassing during sampling with similar methods from other test sections in the evaluated borehole was insignificant
    - 0.5 0.9 Pressure responses during similar hydraulic testing of other test sections in the evaluated borehole indicate insignificant degassing
    - 0.5 0.9 Direct observations of other test sections in the evaluated borehole indicate insignificant degassing
    - 0.5 0.5 0 Comparison with the characteristics of sampling in other test sections in the evaluated borehole indicate insignificant degassing
      - 0.7 0.9 Results from similar sampling locations in other test sections in the evaluated borehole indicate insignificant degassing
      - 0.8 0.9 Behaviour of sampling containers with similar characteristics in other test sections indicate insignificant degassing
  - 0.3 ANY 0 Temperature variations during sampling were insignificant
    - 0.8 0.8 Temperature measurements in surface flow lines
    - 0.9 0.9 Temperature measurements made using downhole sampling tools
    - 0.8 0.8 Measurements made using wireline tools



- 0.5 ANY 0 Chemical processes during sampling from other boreholes were insignificant
  - 0.25 ANY 0 Reaction between groundwater and sampling apparatus was insignificant in other boreholes
    - 0.6 0.7 Direct observations of sampling apparatus indicate no significant reactions
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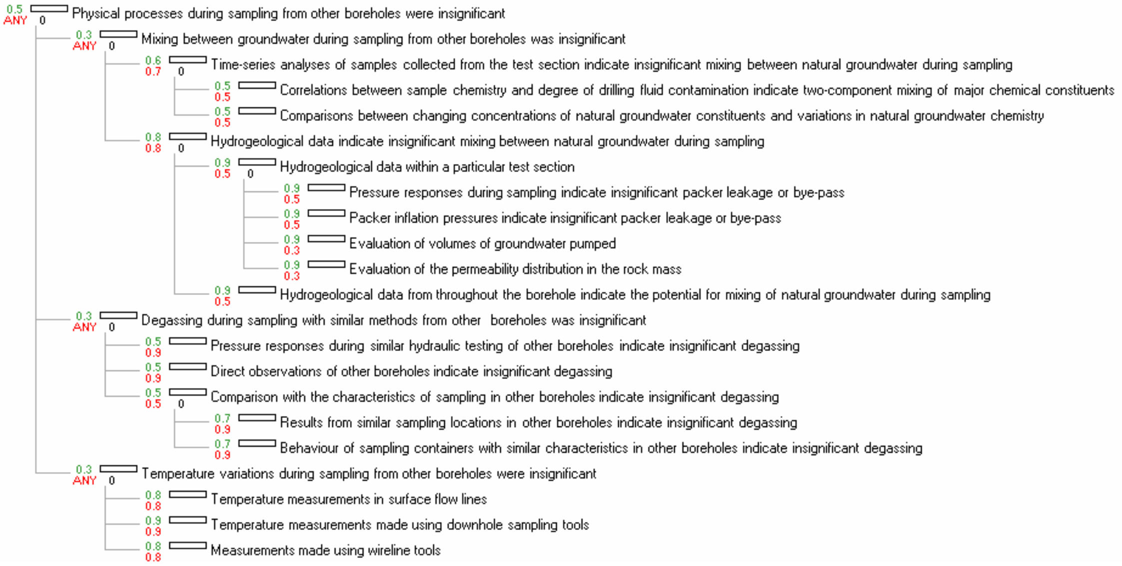

- 0.5 ANY 0 Physical processes during sampling from other boreholes were insignificant
  - 0.3 ANY 0 Mixing between groundwater during sampling from other boreholes was insignificant
    - 0.6 0.7 0 Time-series analyses of samples collected from the test section indicate insignificant mixing between natural groundwater during sampling
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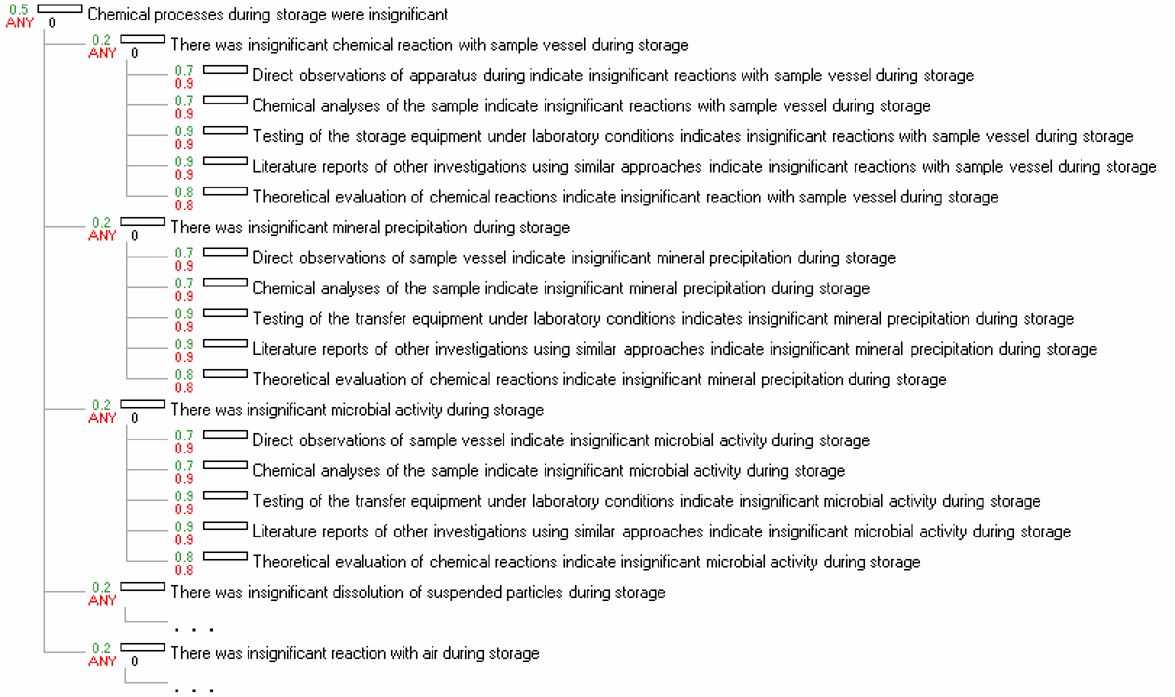
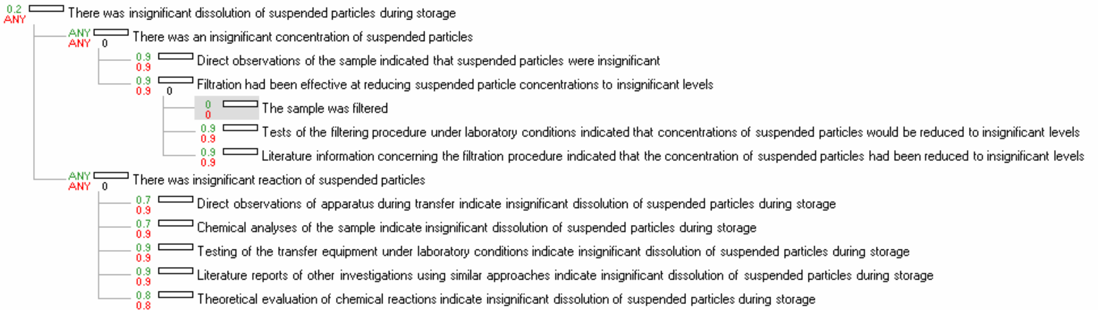
  - 0.3 ANY 0 Degassing during sampling with similar methods from other boreholes was insignificant
    - 0.5 0.9 Pressure responses during similar hydraulic testing of other boreholes indicate insignificant degassing
    - 0.5 0.9 Direct observations of other boreholes indicate insignificant degassing
    - 0.5 0.5 0 Comparison with the characteristics of sampling in other boreholes indicate insignificant degassing
      - 0.7 0.9 Results from similar sampling locations in other boreholes indicate insignificant degassing
      - 0.7 0.9 Behaviour of sampling containers with similar characteristics in other boreholes indicate insignificant degassing
  - 0.3 ANY 0 Temperature variations during sampling from other boreholes were insignificant
    - 0.8 0.8 Temperature measurements in surface flow lines
    - 0.9 0.9 Temperature measurements made using downhole sampling tools
    - 0.8 0.8 Measurements made using wireline tools



- 0.5 ANY 0 Chemical processes during storage were insignificant
  - 0.2 ANY 0 There was insignificant chemical reaction with sample vessel during storage
    - 0.7 0.9 Direct observations of apparatus during indicate insignificant reactions with sample vessel during storage
    - 0.7 0.9 Chemical analyses of the sample indicate insignificant reactions with sample vessel during storage
    - 0.9 0.9 Testing of the storage equipment under laboratory conditions indicates insignificant reactions with sample vessel during storage
    - 0.9 0.9 Literature reports of other investigations using similar approaches indicate insignificant reactions with sample vessel during storage
    - 0.8 0.8 Theoretical evaluation of chemical reactions indicate insignificant reaction with sample vessel during storage
  - 0.2 ANY 0 There was insignificant mineral precipitation during storage
    - 0.7 0.9 Direct observations of sample vessel indicate insignificant mineral precipitation during storage
    - 0.7 0.9 Chemical analyses of the sample indicate insignificant mineral precipitation during storage
    - 0.9 0.9 Testing of the transfer equipment under laboratory conditions indicates insignificant mineral precipitation during storage
    - 0.9 0.9 Literature reports of other investigations using similar approaches indicate insignificant mineral precipitation during storage
    - 0.8 0.8 Theoretical evaluation of chemical reactions indicate insignificant mineral precipitation during storage
  - 0.2 ANY 0 There was insignificant microbial activity during storage
    - 0.7 0.9 Direct observations of sample vessel indicate insignificant microbial activity during storage
    - 0.7 0.9 Chemical analyses of the sample indicate insignificant microbial activity during storage
    - 0.9 0.9 Testing of the transfer equipment under laboratory conditions indicate insignificant microbial activity during storage
    - 0.9 0.9 Literature reports of other investigations using similar approaches indicate insignificant microbial activity during storage
    - 0.8 0.8 Theoretical evaluation of chemical reactions indicate insignificant microbial activity during storage
  - 0.2 ANY There was insignificant dissolution of suspended particles during storage
    - . . .
  - 0.2 ANY 0 There was insignificant reaction with air during storage
    - . . .



- 0.2 ANY There was insignificant dissolution of suspended particles during storage
  - ANY ANY 0 There was an insignificant concentration of suspended particles
    - 0.9 0.9 Direct observations of the sample indicated that suspended particles were insignificant
    - 0.9 0.9 0 Filtration had been effective at reducing suspended particle concentrations to insignificant levels
      - 0 0 The sample was filtered
      - 0.9 0.9 Tests of the filtering procedure under laboratory conditions indicated that concentrations of suspended particles would be reduced to insignificant levels
      - 0.9 0.9 Literature information concerning the filtration procedure indicated that the concentration of suspended particles had been reduced to insignificant levels
  - ANY ANY 0 There was insignificant reaction of suspended particles
    - 0.7 0.9 Direct observations of apparatus during transfer indicate insignificant dissolution of suspended particles during storage
    - 0.7 0.9 Chemical analyses of the sample indicate insignificant dissolution of suspended particles during storage
    - 0.9 0.9 Testing of the transfer equipment under laboratory conditions indicate insignificant dissolution of suspended particles during storage
    - 0.9 0.9 Literature reports of other investigations using similar approaches indicate insignificant dissolution of suspended particles during storage
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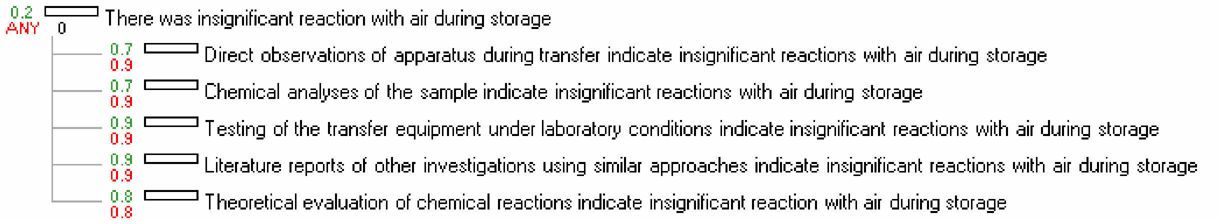

- 0.2 ANY 0 There was insignificant reaction with air during storage
  - 0.7 0.9 Direct observations of apparatus during transfer indicate insignificant reactions with air during storage
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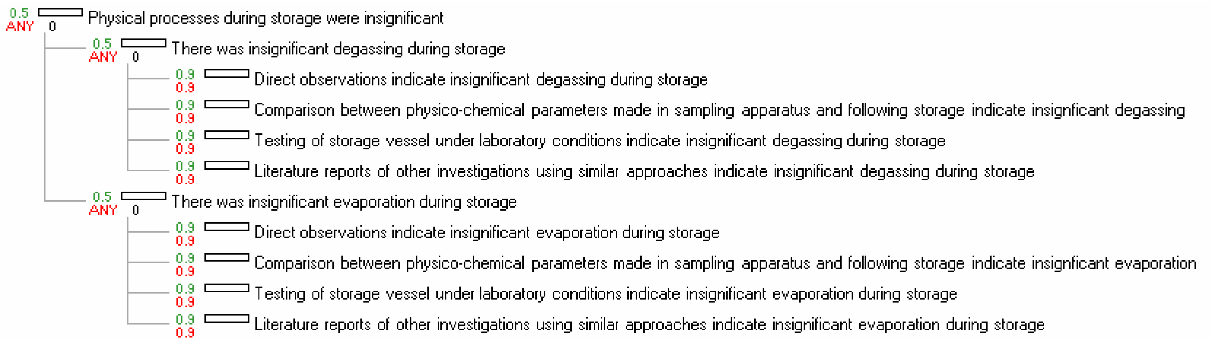

- 0.5 ANY 0 Physical processes during storage were insignificant
  - 0.5 ANY 0 There was insignificant degassing during storage
    - 0.9 0.9 Direct observations indicate insignificant degassing during storage
    - 0.9 0.9 Comparison between physico-chemical parameters made in sampling apparatus and following storage indicate insignficant degassing
    - 0.9 0.9 Testing of storage vessel under laboratory conditions indicate insignificant degassing during storage
    - 0.9 0.9 Literature reports of other investigations using similar approaches indicate insignificant degassing during storage
  - 0.5 ANY 0 There was insignificant evaporation during storage
    - 0.9 0.9 Direct observations indicate insignificant evaporation during storage
    - 0.9 0.9 Comparison between physico-chemical parameters made in sampling apparatus and following storage indicate insignficant evaporation
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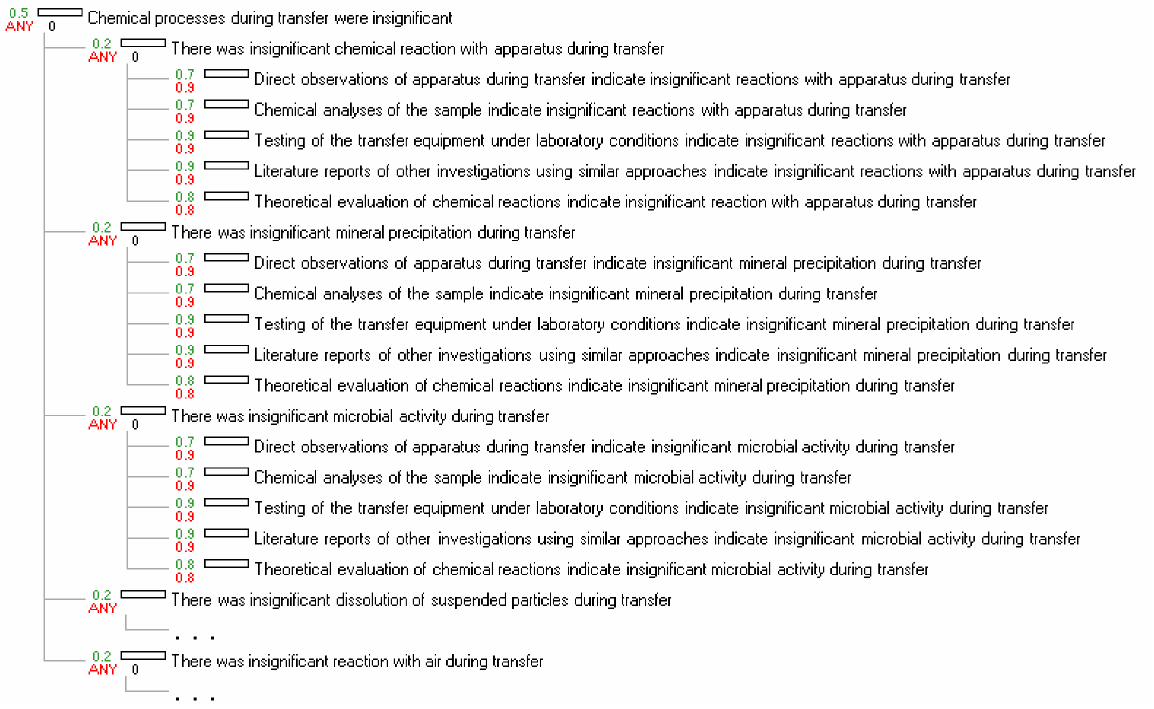

- 0.5 ANY 0 Chemical processes during transfer were insignificant
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    - 0.7 0.9 Direct observations of apparatus during transfer indicate insignificant reactions with apparatus during transfer
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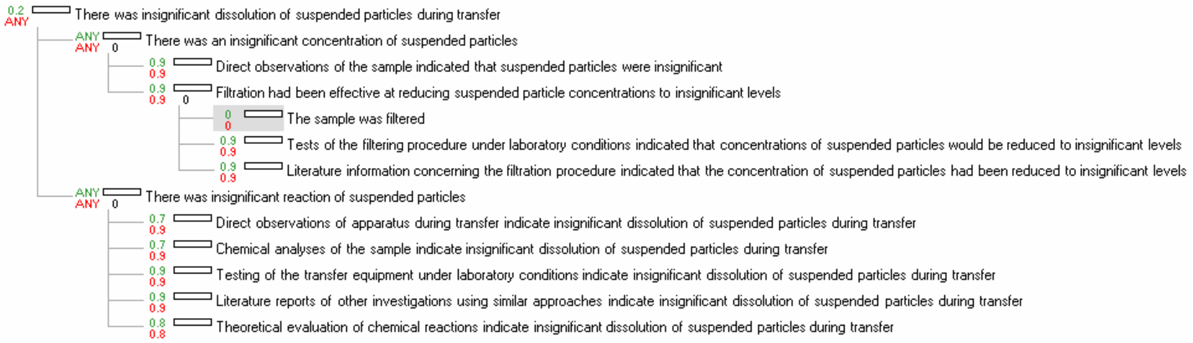
    - . . .
  - 0.2 ANY 0 There was insignificant reaction with air during transfer
    - . . .



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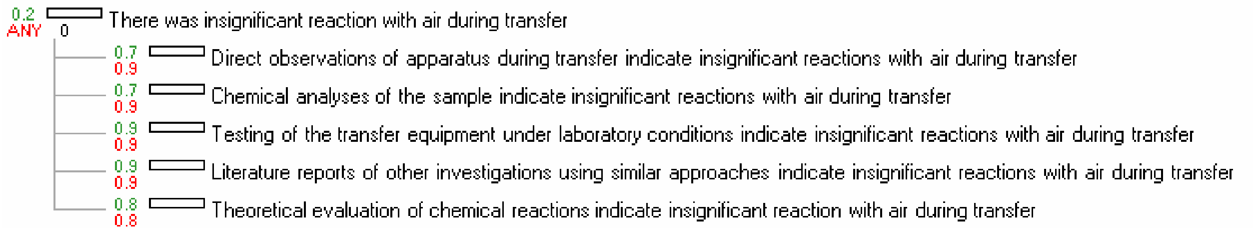

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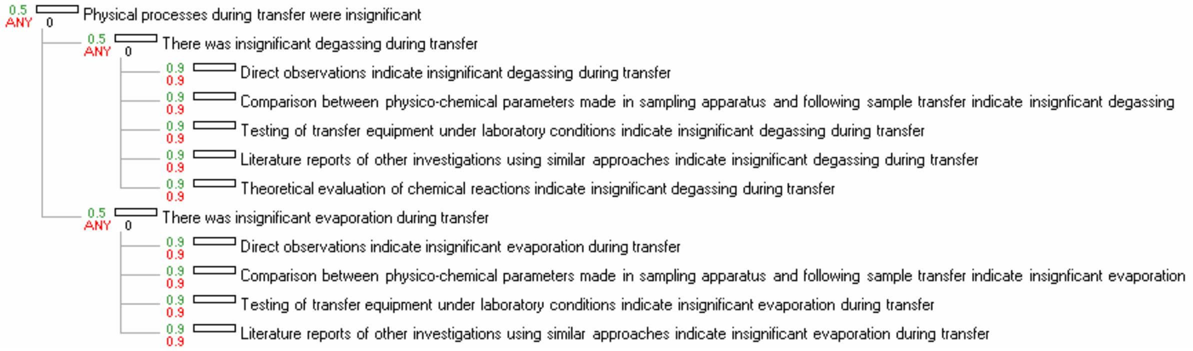

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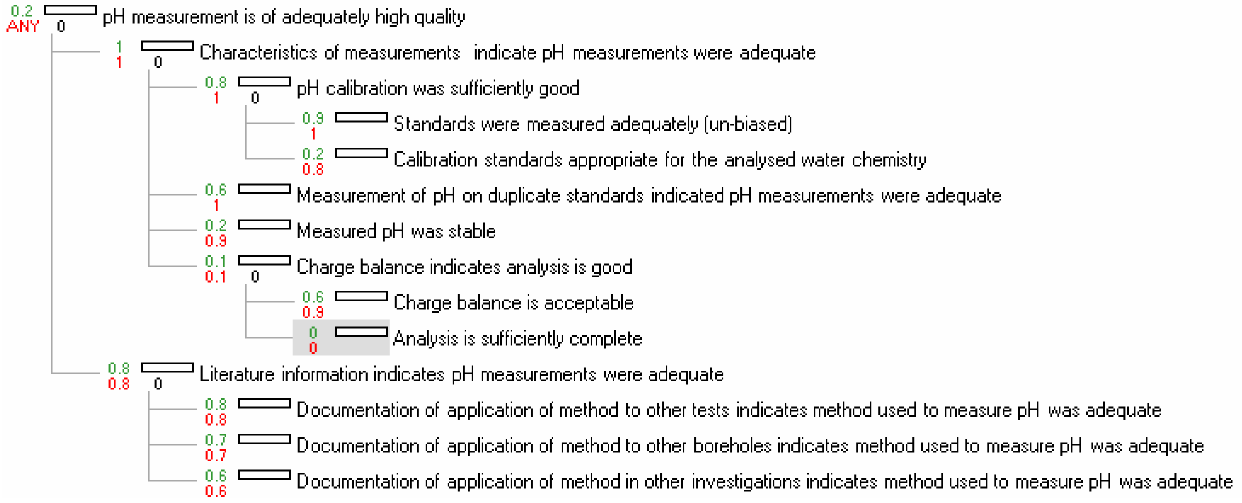

- 0.2 ANY 0 pH measurement is of adequately high quality
  - 1 1 0 Characteristics of measurements indicate pH measurements were adequate
    - 0.8 1 0 pH calibration was sufficiently good
      - 0.9 1 Standards were measured adequately (un-biased)
      - 0.2 0.8 Calibration standards appropriate for the analysed water chemistry
    - 0.6 1 Measurement of pH on duplicate standards indicated pH measurements were adequate
    - 0.2 0.9 Measured pH was stable
    - 0.1 0.1 0 Charge balance indicates analysis is good
      - 0.6 0.9 Charge balance is acceptable
      - 0 0 Analysis is sufficiently complete
  - 0.8 0.8 0 Literature information indicates pH measurements were adequate
    - 0.8 0.8 Documentation of application of method to other tests indicates method used to measure pH was adequate
    - 0.7 0.7 Documentation of application of method to other boreholes indicates method used to measure pH was adequate
    - 0.6 0.6 Documentation of application of method in other investigations indicates method used to measure pH was adequate

Appendix 3 Review comments by Dr A.H. Bath, Intellisci Ltd, on draft process models

1. Overview of draft process models

The process models are a draft contribution to the development of a classification system for the quality of hydrogeochemical data from the Tono area. The process models build on the development by JNC of a quality classification system, including the preliminary scoring scheme developed by Furue (2003). Some comments concerning this previous scheme are added here. The limitations of Furue's scheme are discussed in terms of the available information for scoring and the discrimination of data as being 'fit for purpose'. The main methodological limitations of that scheme are (a) that misleading scores can arise due to compensation of low scores on some quality indications by high scores on other less important indicators, and (b) that the quality indicators do not have consistent or appropriate implications for data quality.

The draft ESL process models aim to implement a more sophisticated approach to assessing data quality that should eliminate the limitations of the simple quality scoring method. This new approach develops Evidence Support Logic (ESL) as a way of capturing and quantifying factual information and expert judgement about the various technical factors that underlie data quality. ESL provides an algorithm for giving appropriate weighting to factors, for relating them in a logical way, and for propagating probability of data quality being 'fit for purpose' and residual uncertainties. Visualisation of the ESL model structure and application of the algorithm is carried out with Quintessa's TESLA software.

Alternative structures of the ESL model are considered that show ways of breaking down the evidence for the top-level proposition about data quality. One way is to break down the information according to technical categories and then within each category (e.g. geochemical, hydrogeological, QC strategies) into specific pieces of information and expert judgements on how these should be weighted and propagated to higher levels in the ESL model. The other way that is illustrated is to breakdown information directly into judgements about specific processes that could perturb measurements. The latter structure of the ESL model is selected for illustrative application to JNC's data from the Tono area. It is then simplified to include only those processes for which information is available. Some examples of how the ESL model might be structured, breaking it down to various levels of detail, have also been provided. Comments on these as illustrations of various points about ESL structure are given here in an appendix.

2. Focus of Review

I have been asked to comment particularly on:

- ▲ the suitability and completeness of proposed quality indicators,
- ▲ the advantages and disadvantages of the ESL method,
- ▲ the structure of the ESL process models,
- ▲ how 'sufficiency' parameters have been derived that govern the propagation of information to higher level processes,
- ▲ the result for assigning values to evidence at the lowest level whereby judgements have to fully one or the other so that they give Boolean values (0 or 1),
- ▲ possible applications of the quality evaluation scheme.

I carried out the review in a sequence of stages:

- ▲ Read the critique of the original quality scheme by Furue (2003) along with my own review (Bath, 2004)
- ▲ Compiled my own summary notes about the key issues for data quality evaluation:
    - the intended purpose for hydrochemical data (i.e. radionuclide solubility and mobility) and thus what are the pertinent 'priority' parameters;
    - the categories of sample and analytical perturbation that might cause data to be unreliable;
    - the types of quality indicator data or other information, whereby some conditions are essential or disqualifying whilst other conditions have a gradational effect on quality and other bits of information have to be used simply as optional contributions to expert judgement.
- ▲ Reviewed the proposed ESL approach, parameterisation rules and illustrate outcomes and compared these with my qualitative summary of key issues and criteria for data quality.
- ▲ Examined the detailed structure and scoring of the provided examples of ESL quality classification.

3. Additional Comments on JNC's Preliminary Scheme

I agree with all of the points made in Section 2.2 in discussing the limitations of the preliminary scheme. The additive method of scoring is the main limitations, because it can 'compensate' poor and potentially disqualifying factors. My previous review (Bath, 2004) has already emphasised the contrast between a quality scoring scheme that is being applied to a homogeneous high-quality data set and the scheme being applied to a heterogeneous and relatively poor data set. The latter case invariably requires both scoring against criteria and expert judgement to rescue information.

As it stands, the preliminary scheme does not explicitly identify data that should be disqualified as not being 'fit for purpose'. The purpose is understood to be the modelling of radionuclide solubilities, for which redox/Eh, pH, TIC, total salinity and DOC are in general the key parameters (SO_4, PO_4, F are possibly of secondary importance). They are key parameters because variations within plausible ranges can cause order of magnitude variations in both solubilities and sorption parameters for some radionuclides. Therefore erroneous values that are plausible and thus not detectable could propagate significant errors into PA modelling.

The most important and most vulnerable to perturbation of these key parameters is Eh/redox. Only slight oxygenation by air contamination is sufficient to cause a step change perturbation of Eh from reducing to oxidising. Therefore a gradational quality scoring system is not appropriate for assessing the validity of Eh in a data set. pH and TIC are also easily perturbed but are less likely to suffer step changes; therefore the scoring system is more appropriate. Moreover there are numerical geochemical methods by which pH and TIC can be evaluated and, in certain cases, adjusted to 'most likely' in-situ values. Salinity has a gradational influence through the ionic strength effect on ion activity, and in the scoring system is also more appropriate. DOC also has a gradational effect on solubility and mobility via formation of organic complexes, but sampling and measurement are subject to specific perturbations that could result in either abnormally high or erroneous zero measurements.

The general point is that each of the key parameters has its own type of sensitivity to perturbation and error, and also that they each have different impacts on solubility and mobility for specific radionuclides. Eh and pH are the most important factors, in general. However Eh/redox only has substantial sensitivity insolubilities and speciation of U and Tc, and to a lesser extent also Np and Pu. Radionuclide solubilities and speciation are more widely affected by pH, especially the actinides that are hydrolysed i.e. form OH complexes. Therefore it has to be said that a quality scoring system, or any attempt at an 'expert system', is fraught with problems unless it has scope for expert judgement to overrule or adjust quality scores (which will tend to compromise the aim of objectivity). These issues should be handled more satisfactorily in the ESL approach to quality screening.

Another by-product of the additive scoring system is that minor 'supplementary' bits of qualitative information of debatable significance may be given too much weight. For some parameters, there may be no relationship or dependence at all. For example, for the key parameters Eh and pH, charge balance on the analyses of major cations and anions has no implications at all for the validity of pH and Eh data. The ESL approach must make this distinction.

A method that improves upon the preliminary scoring system must also optimise the use of data and minimise the discounting of data for lack of formal information where expert judgement and other peripheral information might justify some degree of cautious value.

4. An Independent Opinion of the Key Issues

I summarise here what I think are the key issues and priority data and other information that should be considered in assessing quality of hydrochemical data and their fitness for purpose (as discussed above).

- ▲ What hydrochemical data are the priorities for calculating radionuclide solubilities, speciations and sorption/mobilities?
    - redox condition (Eh, Fe^{2+}/Fe^{3+}, HS^-, O_2 (aq), CH_4)
    - pH (pH, HCO_3^-, DIC, PCO_2)
    - salinity (EC, TDS, Cl-, SO_4^{2-})
    - DOC, colloids, other particulates, microbes, biomass
    - specific ligands (CO_3, PO_4, F)
- ▲ What are the categories of contaminations and chemical perturbations?
    - addition of drilling water (organics, bentonite, other colloids, dilution, pH alteration, reaction with rock 'flour')
    - in-mixing of extraneous formation waters (dilution or salinization, misleading concentration gradients, smoothing of hydrochemical compartmentalisation)
    - out-gassing (loss of CO_2, increased pH, calcite supersaturation and precipitation Fe-ox precipitation, stripping of other gases, e.g. CH_4, H_2S)
    - oxygenation (oxidation, Fe-ox precipitation, oxidation of HS^- and labile organics, oxidation and dissolution of sulphide minerals in rock 'flour' and wall rock)
    - addition of rock 'flour' particles (sorption and loss of sorbed ions by subsequent filtration, dissolution reactions)

- growth of microbial biomass (reduction of DIC, sorption to cellular material, redox changes and precipitation)
- equipment surface effects (sorption of trace elements and Fe, nucleation of precipitation, out-diffusion of gases)
- specific contaminants (drilling water additives, equipment 'memory').

▲ Qualifying and disqualifying conditions for specific parameters

- Eh: drilling fluid contamination must be below a low threshold, must be measured down-hole or in a well-head flow cell, disqualified if sampled by air-lift extraction, stability monitoring needs expert interpretation with respect to buffering and electrode response, disqualified if measured in static open sample and/or in lab.
- pH: drilling fluid contamination must be below a low threshold, expert interpretation of measurements on air-lifted, static or stored samples, generally lower score for lab pH, stability monitoring needs expert interpretation with respect to out-gassing, in-gassing and electrode response.
- Redox-sensitive solutes (esp. dissolved O_2, Fe, S_{red}, U): special preservation of sample for O_2, Fe^{2+} and Fe_{tot} analyses and reduced S analysis, disqualified if air-lifted or oxygenated at any stage of sampling/transfer.
- Salinity and non-reactive major solutes and trace metals: drilling fluid contamination must be below a level at which linear mixing/dilution correction is acceptable.
- DIC, alkalinity, PCO_2: as for pH, considering requirement to demonstrate internal consistency in pH-DIC system.

▲ What additional factors should be considered?

- Pumping rate: too high and too low can be detrimental to sample quality and especially to reliability of pH and Eh monitoring.
- Charge balance: has no direct implications for reliability of Eh, pH and other labile parameters except HCO_3, but is necessary for assessing major ions reliability prior to using geochemical modelling to test consistency of carbonate equilibria and pH.
- Knowledge and stability of drilling water composition including tracer concentration: uncertainty in these is propagated into uncertainty in corrected in-situ concentrations of non-reactive solutes.
- Extraneous formation water: untraced component of water in borehole during drilling, may introduce large uncertainty into corrected concentrations.
- Filtration history of water sample: needs to be considered with knowledge of colloids, organics and particulates, possibility for precipitation prior to or during filtration
- Preservation methods for stabilising specified parameters: Fe^{2+}, HS^- especially if being analysed to support redox interpretation.

- Calibration of electrodes: for pH and Eh measurement.

The preliminary quality scoring system has a maximum score of 6.6, with a contribution of only 3 deriving from assessment of the three dominant criteria for Eh and pH: drilling fluid contamination, Eh-pH measurement locations and methods, and sampling location. In practice, with the Tono area data in Appendix 1, samples from only 7 boreholes were not disqualified on the basis of contamination (using a suggested limit of 5%) and Eh and pH measurement location. These samples are:

Borehole	Quality Score
DH-13	4.07 and 4.38
KNA-6	2.88 to 4.24
DH-12	4.32 and 3.67-4.23
MIU-4	4.54
MSB-2	3.74-4.00 and 3.86
MSB-4	4.21
MIZ-1	2.89 to 4.35

Some other samples have relatively high scores, despite being disqualified on the basis of drilling water contamination or method of Eh & pH measurements. Disqualified samples with scores above 3.2 are:

Borehole	Quality Score	Disqualification cause
DH-4	3.77	Contamination
DH-5	4.23	"
DH-6	4.23	"
DH-7	3.73-3.48	"
DH-8	3.94-3.34	"
DH-9	3.86-4.56	"
DH-10	4.13	"
DH-11	3.75	"
DH-15	4.07	Eh-pH measurement location

Thus the preliminary scoring system fails to identify a number of samples that are probably unreliable for the parameters of interest (Eh and pH), although it generally gives relatively high scores to the most successful samples in these terms.

What this simple exercise shows is that a quality classification system of this type should have a stage where the criteria of dominant importance are screened prior to a more general and additive scoring system.

The ESL method that is being proposed by Quintessa must therefore offer the following basic advantages over the preliminary scoring system:

- Primary screening of the key quantitative criteria for reliability of Eh/redox and pH, namely drilling water contamination and methods of sampling and measurement;
- Non-additive evidence propagation, so that disqualifying or negative factors are not directly compensated by other factors;
- Supplementary information that requires expert judgement can be taken into account but is not given undue weight;
- Methodology and structure can be customised for individual geochemical parameters to accurately reflect their specific sensitivities and significance to PA.

5. Review of the ESL Methodology

Suitability and completeness of proposed quality indicators

Proposed quality indicators are those considered in JNC's preliminary scheme (Furue, 2003):

- degree of drilling water contamination,
- ionic charge balance,
- delay time from sampling to analysis of HCO_3, Fe, Sred,
- sampling container (but not counted in scoring)
- sampling logistics, i.e. downhole, pumped or air-lifted,
- length of sampled interval,
- measurement of pH and Eh, i.e. downhole, surface, lab.
- monitored stability of pH, Eh, EC

plus additional indicators:

- consistency of pH and alkalinity/TIC with calcite equilibrium,
- consistency between Eh and other redox-sensitive indicators i.e. Fe^{2+} & Fe^{3+}, HS^-, CH_4, U,
- completeness of analysis,
- natural tracers of contamination by anomalously young water,
- anomalous or 'odd' chemical composition,
- amount of flush pumping before sampling,
- borehole completion and stabilisation materials and design,
- drilling equipment materials,
- borehole cleaning history,
- information about sampling equipment operation/malfunction
- sample transfer arrangements,
- sample filtration and preservation,
- sample storage conditions,
- consistency among replicate samples and analyses.

This list of quality indictors is fairly comprehensive, though I suggest that two indicators are added: (i) in-mixing of extraneous formation waters, and (ii) evidence from visual examination of water samples.

In-mixing of extraneous formation water, i.e. water that has entered the borehole from outside the sampled interval and in contrast to drilling water is un-traced, has been found to be a major proportion of some water samples taken from deep boreholes in the Swedish site, investigation programme. For example, calculations using tracer monitoring data, drilling water loss volumes, water pressures and hydraulic conductivity logs indicated that only about 19% of the water that had intruded a sampled interval was drilling water (Laaksoharju et al., 2004a,b; SKB, 2004). The 'Drilling Impact Study' methodology developed by SKB should be examined and considered as a monitoring procedure for future borehole drilling and sampling by JNC.

Evidence from visual examination of water samples is a simple and widely-used source of information and judgement about contamination both during sampling and prior to analysis. Amongst the contaminating phenomena that might be detected are:

- ▲ discolouration,
- ▲ colloidal or particulate material,
- ▲ precipitation of Fe-oxide,
- ▲ growth of microbial or algal biomass.

Additionally, if analytical uncertainties are to be included in the quality classification, then I suggest that calibration and performance of electrodes used for Eh and pH measurements should be considered. Analytical, i.e. in-laboratory, impacts on data quality and reliability seem to have been excluded from the proposed scheme at this stage. However, electrode calibration and performance are important factors in field data, especially for downhole probe measurements.

The complete list of indicators is a mixture of quantifiable measurements and qualitative information requiring expert judgement of its significance to quality. The ESL method provides a way of using these judgements, but this has to be done carefully.

5.1 Advantages and disadvantages of ESL method

In my opinion, the ESL method has the great advantage of providing a framework for a systematic and comprehensive interrogation of evidence. It provides a visual and auditable record of the process. Perhaps most importantly, it is a method for capturing and giving appropriate weights to different types of information and avoids the pitfalls of an additive scoring scheme.

The most obvious disadvantage, I think, is that it appears to be excessively laborious for a set of expert judgements that can be made more simply. Such judgements are made routinely during all similar site investigations and interpretations, and probably have a similar robustness despite being more 'ad hoc'. An illustration of this is provided by the discussion of quality scoring for the Tono area data, in Section 3.2. For the parameters of interest, drilling fluid contamination and measurement method are the two overriding criteria for reliability. ESL represents this in the 'Any' designation for sufficiency of evidence against (see Fig. 3 9) whereas Quality Scoring does not, but it can be argued that the complexity of the ESL model construction is not necessary to make judgements on these criteria.

The ESL approach is ideally suited to discussion making or proposition testing where the top-level proposition is supported or tested by very diverse lines of evidence on which expert opinions might vary. The relative simplicity of some of the points of evidence for sample quality is indicated by the use of a Boolean variable (1 or 0, yes or no) in many cases.

5.2 Structure of the ESL model

Alternative structures of the ESL model are illustrated – one broken down into processes grouped according to type of information (Figure 3-8) and the other broken down according to list of potential perturbations on the parameter of interest, pH (Figure 3-9). The two become very similar in terms of judgements at the lowest-level nodes. The second structure is more complex and comprehensive because it systematically interrogates against each quality indicator in the extended list (see above). A potential problem is that having so many nodes, each of which might disqualify the sample/data, raises the chance of having a disqualification on strong or weak grounds depending on available information and expert judgement.

In summary, the inclusion of all possible evidence in the second structure (Figure 3-9), including inferences from indirect evidence such as observations in other boreholes, produces a checklist with too many disqualifying possibilities if used rigorously. Alternatively, use of the structure with more flexibility mimics what is involved in normal expert judgement without the ESL model.

An additional comment on the way that ESL is implemented in this application is that assessments of the low-level nodes are likely to be made by a solo expert, whereas ESL is most effective for capturing a spread of opinions or interpretations on each process. Again, this raises the question of whether the ESL procedure is too laborious.

The simplified structure of the ESL model that includes only low-level processes for which information exists (Appendix 2, first diagram) is a logical development that recognises the limitations on information. It can be criticised as avoiding judgements on the implications of missing information that could, in a few cases, be very significant. These 'one-off' cases where information is being rescued from samples or data that are unreliable for specific reasons are perhaps better considered by application of expert judgement without the rigid framework of ESL. An example of this would be systematic operator error in the operation of the pH meter or electrode, which would not be considered in the strict adherence to the simplified diagram in the appendix.

A distinct advantage of the simplified structure in Fig 3-10 is that the status of 'Any' for sufficiency against is reserved for the second-highest level processes. Lower level processes have variable parameterisation of sufficiencies, thus allowing more flexibility in the ESL procedure and its outcome.

I suggest that charge balance should be removed from the overall model presented in Appendix 2, since it does not indicate anything about pH reliability. I also suggest that calculated PCO_2 should be added as a source of evidence, i.e. log PCO_2 <-3.5 is probably not outgassed, >-3.5 indicates a tendency to outgas, = 3.5 has probably already outgassed to equilibrium with air.

5.3 Derivation and evaluation of 'sufficiency' parameters

Sufficiency parameters have been derived by assigning values of 1 alternately for and against the lowest-level process, and then propagating these upwards to the second-highest process.

The top-level and second-highest level processes in the overall model present in Appendix 2 are null hypotheses, i.e. any evidence of a perturbing effect rejects the proposition. It is therefore inevitable that the sufficiencies 'against' the low-level processes will be high values, and the sufficiencies 'for' will be low values. The question arises of whether sufficiencies against should have values of 1. But these low-level processes are mostly observations (e.g. 'degree of contamination by drilling water', 'volumes of drilling return fluid') that have only indirect, interpreted, implications for impact on pH. Essentially their impacts are gradational and require expert judgement. Therefore values of 1 would be in appropriate.

Overall, the ESL visualisation (as in the overall model in Appendix A) does not indicate how the sufficiency values have been assigned at the lowest level and then propagated to higher levels. In effect, the expert judgement lying behind this lacks transparency just as does expert judgement used in normal interpretations.

The ratio of 'evidence for' to 'evidence against' propagated through Fig 3-10 to the top-level proposition regarding pH reliability is said to be 2.4, with residual uncertainty of 0.6. How has the ratio of 2.4 been calculated? This value seems counter-intuitive considering that only one of the low-level processes has evidence against it, with a sufficiency weighting of only 0.12. Presumably, the relatively large contribution of uncertainty is part of the explanation. In the example, the 'evidence against' appears to originate from too little flushing before sampling. What implication this information has is a matter of expert judgement, and it's not evident that the weight accorded to this in ESL is appropriate. Thus a potential challenge to data reliability would come down to the role of expert opinion, and it's arguable whether ESL makes the matter any more transparent.

5.4 Rules for assigning Boolean values to quality indicators

I agree with the simplification of scoring on these low-level quality indicators to Boolean values, i.e. yes or no. Any other scheme of graded severity would be too subjective and not transparent, even if more 'adaptive' to circumstances. Lack of knowledge scores as zero.

The criteria for success/failure, or yes/no, applied in the draft model presented in Appendix 2 are summarized in Table A3-1. These criteria involve sophisticated reasoning. For example, flush-pumping before sampling is evaluated on the basis of comparing the volume of removed water with the scale over which groundwater compositions might vary. But SKB's Drilling Impact Studies indicate that large volumes have to be pumped out to get to an acceptably low level of contamination by drilling water. Thus the reality of optimising flush-pumping is a compromise which is not really reflected by the criterion in Table A3-1. Equally, SKB's DIS shows that a decision on what volume of drilling water loss becomes significant should involve a complex analysis of several types of data.

Table A3-1 Rules for assigning 'evidence for' and 'evidence against' each process corresponding to a data quality indicator in the simplified data process model (Appendix 2).

Quality indicator	Criteria for success/failure
Degree of contamination by drilling water, as indicated by fluorescent dye insignificant	If the contamination is <1%, then the evidence for is 1; if >1% the evidence against is 1
Degree of contamination by drilling water, as indicated by natural tracers	If contamination is undetectable, then the evidence for is 1; if detectable the evidence against is 1
Characteristics of borehole completion (e.g. whether cemented or not) favourable	If no artificial materials were used, then the evidence for is 1; if cementing was employed, the evidence against is 1
Characteristics of drilling equipment favourable	If the drilling equipment would not corrode, then the evidence for is 1; if corrosion could occur then the evidence against is 1
Characteristics of loss-control materials favourable	If reactive loss-control materials were used, then the evidence for is 1; if these materials were not used, then the evidence against is 1
Volumes of drilling return fluid	If the volumes of drilling return fluid indicate insignificant drilling fluid loss, then the evidence for is 1; if there was significant drilling fluid loss, then the evidence against is 1
Characteristics of borehole cleaning materials favourable	If reactive borehole cleaning fluids were not used, then the evidence for is 1; if reactive borehole cleaning fluids were used, then evidence against is 1
Sample container unreactive	If the sample container was unreactive, then the evidence for is 1; if it was reactive, then the evidence against is 1
Sample container adequately sealed	If the sample container was adequately sealed, then the evidence for is 1; if it was not adequately sealed, then the evidence against is 1
Stability of physico-chemical parameters	If the physico-chemical parameters have changed by < 5%, then the evidence for is 1; if > 5% then the evidence against is 1
Sampling locality inhibits perturbation	If the sample was collected downhole, then the evidence for is 1; if it is collected at the surface, then the evidence against is 1
Amount of water pumped before sampling	If the water pumped from the test section before sampling was insufficient to draw water over a distance comparable to the spatial scale over which groundwater chemistry varies, then the evidence for is 1; if the distance was comparable to, or greater than, the spatial scale over which groundwater chemistry varies, then the evidence against is 1
Storage container unreactive	If the storage container was unreactive, then the evidence for is 1; if it was reactive, then the evidence against is 1
Storage container adequately sealed	If the storage container was adequately sealed, then the evidence for is 1; if it was not adequately sealed, then the evidence against is 1
The pH did not change during water transfer to the measurement apparatus (either from a sample vessel or directly from a flow line)	If the pH in the lab is within 2.5% of the pH measured in a flow-through cell, then evidence for is 1; if the pH measured in the lab differs by >2.5% of the pH measured in the flow-through cell, then evidence against is 1
Stability of pH measurement	If the pH measurement varied by <±2.5%, then evidence for is 1; if the pH measurement varied by >±2.5%, then the evidence against is 1
Charge balance is acceptable	If the charge balance is within 5%, then the evidence for is 1; if it is >5%, then the evidence against is 1
Analysis is sufficiently complete	If the analysis includes all major constituents of typical groundwaters, then the evidence for is 1; if one or more of these major constituents are absent, then the evidence against is 1

Another example is the assessment of whether pH has been affected by sample transfer. Comparing a flow-through pH with a lab pH is useful, but only to the extent that good agreement confirms the validity of the flow-through value. But the flow-through pH will always be preferred over the lab value, so this criterion isn't a sensible yes/no test for the flow-through pH.

Charge balance is not a direct test of the validity of pH, as mentioned previously, although it provides an evaluation of major ions data prior to geochemical modelling of the consistency of pH with carbonate equilibria. Therefore a value of 1 on this criterion would be false support for a pH value (and also for Eh). The same comment applies to completeness of analysis.

For evaluation of pH, Eh and dissolved O_2 data, calibration and zero-testing (for a DO probe) are important criteria for data quality. They should be added to the list.

It is noteworthy that one reason for erroneous Eh values in archived data is that measured potentials were never adjusted for reference electrode potential (which adds about 240-250 mV to measured potential for the normal reference electrode system). There perhaps should be an assessment of the degree of confidence in that adjustment having been done.

In general, data transcription errors are a fairly common cause of erroneous data. Whilst this is indirectly considered under the test for 'anomalous or odd data', there should be a systematic examination for transcription errors, with backwards tracing of values if appropriate.

In the 5th item of Table 4-1, concerning characteristics of loss-control materials, the criteria for success and failure are in error and should be reversed.

5.5 Possible applications of the quality evaluation scheme

The possible applications listed in Section 5 are:

- ranking samples according to their evidence ratios,
- ranking samples according to the degree of uncertainty about data quality
- highlighting data that are or are not reliable for use in PA,

· determining the main causes of uncertainty in data quality, using a series of sub-trees as exemplified in the ESL visualisations in Appendix 2.

The 'audit trail' feature of ESL is an important asset for these applications. However the apparent lack of transparency in how the evidence ratio of 2.4 in the example overall model in Appendix 2 has been derived is a challenge to this asset of ESL. There needs to be some visibility of the algorithm used to propagate judgements through the ESL model.

It is not apparent why the maximum weight on 'evidence for' is only 0.33 if the lower-level processes are all satisfactory. The ESL method appears to be down-grading good data. I do not consider that there is 'always a large uncertainty in the suitability of a particular pH value for use in PA'. Good data are just that – reliable and fit for purpose, especially in PA where the tolerance for pH and most if not all hydrochemical data is n reality fairly wide. Eh is perhaps the most problematic parameter because if can so easily suffer a step change when perturbed that has a substantial significance in PA.

6. Summary

I am impressed by the framework and visualisation that ESL (and the proprietary computer program TESLA) offers for assessing evidence for a proposition. This development of a robust method for screening the quality of groundwater chemistry data makes good use of ESL's ability to handle different types of information with propagation of weighted evidence, dependency and sufficiency. The above discussion has emphasised the importance of being able to take account of, and give appropriate weights to, qualitative and quantitative information including expert judgements. The ESL methodology is superior to a simple additive quality scoring system in terms of rigour and defensibility. However it may, in many cases, end up with similar or identical outcomes in terms of what are the most reliable samples and data. This may be often be the case because, especially for the most sensitive and important parameters of pH and Eh, there are just two or so dominant 'first rank' criteria for high quality. These criteria are contamination by drilling or extraneous borehole water and method of sampling and measurement.

The ESL methodology is best suited to large data sets, collected under well-controlled QC protocols so that there is abundant and well-documented supporting information.

Perhaps most importantly, the ESL methodology and this analysis of the evidence structure provide an extremely valuable framework for planning and prioritising future data acquisition.

7. References

Bath, A, 2004. Review of Quality Scoring System used by JNC on Groundwater Chemistry Data from Tono Research Area. Report for Quintessa K.K., Intellisci, Loughborough.

Laaksoharju, M. et al., 2004a. Hydrogeochemical evaluation of the Forsmark site, model version 1.1. SKB Report R-04-05

Laaksoharju, M. et al., 2004b. Hydrogeochemical evaluation of the 'Simpevarp area, model version 1.1. SKB Report R-04-16

SKB, 2004. Hydrogeochemical evaluation for Simpevarp model version 1.2. Preliminary site description of the Simpevarp area. SKB Report R-04-74.

Appendix: Comments on examples of ESL model structures

A number of different structures for ESL models have been provided as illustrations of different levels of detail and different approaches to breaking down the lines of evidence. They all are based on the proposition that 'pH has not changed significantly from in-situ value'.

The examples are: (all prefixed by 'JNC 2129 pH unchanged'):

1) all 290105 vpmsl (a complete model)

2) chm sto 250105 vpms1 (chemical procs during storage)

3) chm turns 250105 vpms1 (chem. procs during transfer)

4) global 250105 vpms1 (simplified model with conflict in evidence)

5) mix df 250105 vpms2 (mixing with drilling fluid)

6) mix gw 250105 vpms1 (mixing with natural gws)

7) Obh smpl 250105 vpms1 (observations in other test sections)

8) ph evl 310015 vpms1 (simplified model)

9) phys sto 250105 vpms1 (physical processes during storage)

10) phys trns 250105 vpms1 (physical processes during transfer)

11) rxn bhs 250105 vpms1 (reaction with stabilisation material)

12) rxn cls 250105 vpms1 (reaction with bh cleaning fluid)

13) rxn de 250105 vpms1 (reaction with drilling equipment)

14) rxn df 250105 vpms1 (reaction with drilling fluid)

15) rxn LCM 250105 vpms1 (reaction with LCM)

16) sct smpl 250105 vpms1 (observations in test section)

17) tmp d 250105 vpms1 (temperature variations during drilling)

These examples illustrate the difficulties that arise if the processes are decomposed to the level of detail that comprises single actions or pieces of evidence. The basic problem is that the complexity does not result in easier Boolean decisions – in fact, it multiplies almost exponentially the number of expert judgements. The chance of negative assessments being propagated upwards disproportionately, bearing in mind the basic problem of a null hypothesis being tested, probably increases.

They also illustrate the problem of transparency in the parameterisation of the ESL model. Why are so many of the sufficiencies 'against', and in some cases 'for', given sufficiencies of 0.9 or 0.8? Are these well-based and defendable, or are they the only values that allow the ESL model to work plausibly? Parameterisation like this look artificial or even fudged, unless a logical justification can be provided. That would make the thing even more laborious and hardly more credible.

The simplified models are surely the only sensible way to construct ESL for this sort of evaluation exercise.

Model 9 (pH eval) illustrates how the significance of conflicting lines of evidence (for effects on pH during sampling) and the resulting 'parent' process are very sensitive to the sufficiency parameterisation of respective lines of evidence. Model 4 (global) gives an example of outright conflict of evidence in this situation could be quite common in an ESL model that was fully populated with information and expert judgement. It is good that the ESL visualisation shows that conflict exists, but in practice it will have to be resolved by expert judgement.

Appendix 4 Groundwater analyses evaluated, data quality indicators and data quality classification

The data and quality information presented in the following tables came from the following sources:

- EXCEL file 'gwchem2003Dec22.xls' received from JNC on 22nd December 2003;
- EXCEL file 'MIZ1 GW chem sum.xls', received from JNC on 10th November 2004;
- EXCEL file 'DH-15 GW chem sum.xls', received from JNC on 10th November 2004;
- EXCEL file 'MIU-4 GW chem sum.xls', received from JNC on 8th May 2002.

The majority of the information comes from the first of these sources, which contained a tabulation of the quality information used during the development of the preliminary quality ranking scheme.

Table A4-1 Analyses of groundwater samples for which quality has been evaluated during the development of the quality classification scheme.

Index	Location	Depth			Elevation		Sampling or Analyzing	Temp.	pH	Eh(pt)	Eh (Au)	cond.	DO	Na^+	K^+	Ca^{2+}	Mg^{2+}	Sr^{2+}	TC
		Min	Middle	Max	Min	Max													
Units		mbgl	mbgl	mbgl	masl	masl	Date	degC		mv	mv	mS/m		ppm	ppm	ppm	ppm	ppm	ppm
AKEYO F.																			
168	MSB-4	15.8	20.75	25.7	198.7	188.8	2002.11.9		7.5			39		24.5	2.41	50.6	9.72		
169	MSB-4	34.8	48.5	62.2	179.7	152.3	2002.11.9		7.9			42		47.0	2.64	38.1	5.45		
	MSB-4	15.8	20.75	25.7	198.7	188.8	2003.3.10		7.3			36		19.6	2.16	47.4	7.55	0.23	
	MSB-4	26.5	30.2	33.9	188.0	180.6	2003.3.11		8.1			41		29.1	2.33	45.0	6.38	0.21	
	MSB-4	34.8	48.5	62.2	179.7	152.3	2003.3.11		7.9			40		43.6	2.52	38.5	4.96	0.17	
	DH-15	63.0	67.75	72.5			2003.10.10	20.8	8.8	45	73	38		58.3	1.6	3.2	0.4	<0.3	28
	DH-15	84.5	91	97.5			2003.10.4	21.6	9.1	-36	-44	39		65.4	1.1	2.4	0.2	<0.3	29.2
TOKI LIGNITE BEARING F. (LOWER)																			
1	KNA-6 sed.	-			143.0		1995.7.26		9.5			20.2		45.5	0.38	1.70	0.03	<0.01	
2	KNA-6 unconf.	-			136.0		1996.2.16		9.2	-360		18.0		42.5	0.25	2.34	0.02	<0.01	
2	KNA-6 unconf.	-			136.0		1997.12.18		9.4			16.7		46.5	0.24	1.85	0.02	<0.01	20.7
150	DH-12	157.5	160.79	164.1	-20.1	-26.7	2000.7.26	27.1	9.7	-42		40.7		72.5	0.44	2.08	<0.2	<0.3	12.2
159	MIU-4	71.5	74.11	76.8	145.5	140.2	2000.7.24	23.7	9.4	-88		15.7		49.8	0.20	1.44	<0.1	<0.2	
164	MSB-2	79.0	104.75	130.5	119.5	68.0	2002.7.7	21.8	9.1	-118		-		107	0.23	15.00	0.18	<0.3	7.6
165	MSB-2	132.0	142.99	154.0	66.5	44.5	2002.6.29	21.3	8.8	-75		-		130	1.90	27.00	0.11	<0.3	4.8

Table A4-1 continued.

Index	Location	Depth			Elevation		Sampling or Analyzing	Temp.	pH	Eh(pt)	Eh (Au)	cond.	DO	Na$^+$	K$^+$	Ca^{2+}	Mg^{2+}	Sr^{2+}	TC
		Min	Middle	Max	Min	Max													
Units		mbgl	mbgl	mbgl	masl	masl	Date	degC		mv	mv	mS/m		ppm	ppm	ppm	ppm	ppm	ppm
TOKI GRANITE																			
3	KNA-6 gra.	-			121.0		1996.2.16		8.2	0		18.0		29.3	0.43	12.26	0.18	0.08	24.5
3	KNA-6 gra.	-			121.0		1997.12.18		8.5			15.5		31.5	0.50	11.65	0.19	0.08	20.1
170	DH-2	207.5	208.5	209.5	-13.9	-15.9	2002.9.23	24.2	8.5	-60		48		76.0	1.09	15.1	0.20		12.3
171	DH-2	228.5	232.75	237.0	-34.9	-43.4	2002.10.9	22.4	8.7	-46		53		99.5	0.97	17.6	0.17		10.8
172	DH-2	302.7	303.7	304.7	-109.1	-111.1	2002.9.25	22.5	8.7	0		65		98.5	0.96	19.2	0.12		3.9
173	DH-2	305.6	306.55	307.6	-111.9	-113.9	2002.9.10	23.5	8.8	-61		63		88.6	0.56	16.5	0.10		7.1
174	DH-2	309.7	310.7	311.7	-116.1	-118.1	2002.9.17	23.2	8.8	-19		65		91.0	0.64	22.1	0.12		7.1
175	DH-2	313.0	314	315.0	-119.4	-121.4	2002.9.20	24.7	8.7	-99		66		97.0	0.62	21.7	0.11		7.3
176	DH-2	320.9	324.65	328.4	-127.3	-134.8	2002.10.6	23.2	8.6	-103		66		103	0.65	19.9	0.12		7.2
177	DH-2	347.8	348.8	349.8	-154.2	-156.2	2002.9.27	23.7	8.7	-32		77		117	0.64	25.5	0.10		5.5
178	DH-2	365.5	366.5	367.5	-171.9	-173.9	2002.10.1	24.6	8.8	-121		78		114	0.60	25.3	0.10		5.1
179	DH-2	439.5	443.75	448.0	-245.9	-254.4	2002.10.12	23.2	8.8	-60		88		141	0.86	36.3	0.12		4.7
180	DH-2	451.2	455.45	459.7	-257.6	-266.1	2002.10.15	25.0	8.7	-122		103		157	1.00	42.1	0.19		4.4
	DH-7	438.0	441.25	444.5	-97.8	-104.3	1999.5		8.9	-		9.78		7.7	1.56	11.9	0.70		
	DH-7	479.0	482.25	485.5	-138.8	-145.3	1999.6		10.3	-		13.3		13.3	2.49	13.7	0.24		
	DH-7	479.0	482.25	485.5	-138.8	-145.3	2000.7		9.9	-		13.4		18.6	2.36	9.25	0.03		
108	DH-7	560.5	563.75	567.0	-220.3	-226.8	1998.4.20 22	26.2	10.1	-400		17.9		25.4	2.30	5.4	0.31	0.08	21
	DH-7	560.5	563.75	567.0	-220.3	-226.8	1999.7		10.4	-		19.2		20.4	3.65	13.0	0.01		
	DH-7	560.5	563.75	567.0	-220.3	-226.8	2000.8		10.1	-		13.1		19.0	2.42	10.6	0.01		

Table A4-1 continued.

Index	Location	Depth			Elevation		Sampling or Analyzing	Temp.	pH	Eh(pt)	Eh (Au)	cond.	DO	Na$^+$	K$^+$	Ca^{2+}	Mg^{2+}	Sr^{2+}	TC
		Min	Middle	Max	Min	Max													
Units		mbgl	mbgl	mbgl	masl	masl	Date	degC		mv	mv	mS/m		ppm	ppm	ppm	ppm	ppm	ppm
	DH-7	598.0	601.25	604.5	-257.8	-264.3	1999.8		10.8	-		25.0		27.2	3.40	20.3	0.01		
	DH-7	598.0	601.25	604.5	-257.8	-264.3	2000.9		10.8	-		20.2		28.8	2.84	18.2	<0.01		
	DH-7	660.0	663.25	666.5	-319.8	-326.3	1999.9		10.1	-		15.3		18.6	1.63	13.5	0.29		
	DH-7	660.0	663.25	666.5	-319.8	-326.3	2000.10		9.6	-		17.5		30.8	0.96	10.2	0.01		
	DH-7	735.5	738.75	742.0	-395.3	-401.8	1999.10		11.1	-		32.3		40.7	5.72	20.0	0.02		
	DH-7	735.5	738.75	742.0	-395.3	-401.8	2000.11		11.2	-		30.7		45.6	4.58	18.8	0.02		
109	DH-7	833.5	836.75	840.0	-493.3	-499.8	1998.4.2 9	29.3	9.6	-373		29.8		31.3	9.10	3.2	0.58	0.06	22
	DH-7	833.5	836.75	840.0	-493.3	-499.8	1999.11		10.7	-		23.7		40.6	1.92	8.2	0.04		
110	DH-7	880.0	883.25	886.5	-539.8	-546.3	1998.3.11 19	30.9	9.4	-355		29.7		48.0	22.0	5.4	0.71	0.06	25
	DH-7	880.0	883.25	886.5	-539.8	-546.3	1999.12		10.5	-		23.5		46.0	4.2	9.7	0.14		
	DH-7	880.0	883.25	886.5	-539.8	-546.3	2000.12		10.7	-		24.9		49.0	3.7	10.0	0.07		
151	DH-12	171.8	225.99	280.2	-34.4	-142.8	2000.8.27	25.6	9.3	-26		35.8		55.2	<0.2	6.47	<0.2	<0.3	6.56
155	DH-12	431.4	451.96	472.5	-294.0	-335.1	2000.11.22	26.5	9.2	-20		42.3		66.0	0.41	10.4	<0.2	<0.3	6.32
156	DH-12	388.9	409.29	429.7	-251.5	-292.3	2000.12.7	25.7	8.9	-24		77.7		94.9	0.89	32.4	<0.2	<0.3	4.35
157	DH-12	345.9	366.54	387.2	-208.5	-249.8	2000.12.19	25.2	8.9	-84		63.0		81.5	0.91	25.6	<0.2	<0.3	4.39
158	DH-12	279.4	312.04	344.7	-142.0	-207.3	2000.12.27	22.4	9.2	-32		50.4		71.7	0.41	13.1	<0.2	<0.3	5.69
160	MIU-4	82.3	99.37	116.5	134.7	100.5	2000.8.13	22.8	9.2	-304		14.8		47.0	0.24	3.26	<0.1	<0.2	
161	MIU-4	272.8	273.62	274.5	-55.8	-57.5	2000.12.2	20.1	9.4	75		23.0		43.8	0.59	3.44	<0.1	<0.2	
162	MIU-4	505.8	533.09	560.4	-288.8	-343.4	2001.7.2	22.3	9.2	17		13.9		45.0	0.40	3.81	<0.1	<0.2	
163	MIU-4	653.4	668.84	684.3	-436.2	-422.3	2001.8.1	22.5	9.2	-45		14.7		47.6	0.47	4.52	<0.1	<0.2	

Table A4-1 continued.

Index	Location	Depth			Elevation		Sampling or Analyzing	Temp.	pH	Eh(pt)	Eh (Au)	cond.	DO	Na^+	K^+	Ca^{2+}	Mg^{2+}	Sr^{2+}	TC
		Min	Middle	Max	Min	Max													
Units		mbgl	mbgl	mbgl	masl	masl	Date	degC		mv	mv	mS/m		ppm	ppm	ppm	ppm	ppm	ppm
166	MSB-2	171.5	173.49	175.5	27.0	23.0	2002.7.22	20.5	8.6	-140		-		110	1.10	27	0.23	<0.3	6.0
167	MSB-4	95.5	97.25	99.0	119.0	115.5	2002.8.13	23.0	8.8	-86		-		74	0.23	14	<0.1	<0.3	10.0
	MIZ-1	113.1	114.67	116.3			2003.4.20	19.6	9.2	-71		352		59	0.3	5.9	<0.1	<0.3	10
	MIZ-1	215.0	220.34	225.7			2003.7.9	22.3	8.9	-280		480		68	0.9	11	<0.1	<0.3	9.4
Units		mabh	mabh	mabh				degC		mv	mv	mS/m	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l
TOKI GRANITE																			
	MIZ-1	580.80	588.95	597.10			8:00, 10th April 2004	17.5	8.9	-61		65.1	0.0	110.0	1.2	23.9	<0.1	<0.3	
	MIZ-1	649.00	687.48	725.96			9:00, 30th May 2004	23.4	8.7	-25	-32	94	0.0	114.4	1.6	52.4	<0.1	0.6	
TOKI LIGNITE BEARING F. (LOWER)																			
	DH-15	102.70	118.2	133.70			2003/11/15 14:30:00	21.7	10.0	-118		42	0.00	68	0.6	3.7	<0.1	<0.3	
	DH-15	152.10	184.27	216.43			2003/11/2 17:00:00	24.1	9.4	-140	-140	48	0.00	70	0.4	4.0	<0.1	<0.3	
TOKI GRANITE																			
	DH-15	233.55	236.78	240.00			2003/11/29 18:00:00	23.7	8.9	-155	-132	100	0.00	118	0.7	30.1	<0.1	<0.3	
	DH-15	437.60	449.85	462.1			14:00, 4th June 2004	22.5	8.7	-85.3		71	0.00	115	7.7	24.9	0.2	<0.3	
	DH-15	575.50	587.75	600.00			13:00, 18th June 2004	22.7	8.2	-117		141	0.00	200.3	3.9	58.8	0.2	<0.3	
	DH-15	765.00	773.25	781.5			8:00, 25th May 2004	18.4	8.4	-63.4		262	0.00	214	3.9	249.7	0.4	<0.3	

Table A4-1 continued.

Index	**Location**	**Depth**			**Elevation**		**Sampling or Analyzing**	**Temp.**	**pH**	**Eh(pt)**	**Eh (Au)**	**cond.**	**DO**	**Na^+**	**K^+**	**Ca^{2+}**	**Mg^{2+}**	**Sr^{2+}**	**TC**
		Min	**Middle**	**Max**	**Min**	**Max**													
Units		**mbgl**	**mbgl**	**mbgl**	**masl**	**masl**	**Date**	**degC**		**mv**	**mv**	**mS/m**		**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	DH-15	937.00	945.25	953.50			13:00, 12th May 2004	24.3	8.1	-95.5		295	0.00	218	5	322.2	0.4	<0.3	
	DH-15	987.00	995.25	1003.5			14:00, 2th May 2004	23.1	8.5	-80		525	0.00	383	4.3	631	<0.1	<0.3	

Table A4-1 continued.

Index	Location	Depth			IC	TOC	CO_3^{2-} 1)	HCO_3^- 1)	alk.	SO_4^{2-}	HS^-	S^{2-}	F^-	Cl^-	NO_2^-	NO_3^-	Br^-	I^-	NH_4^+
		Min	Middle	Max															
Units		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	meq/l	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
AKEYO F.																			
168	MSB-4	15.8	20.75	25.7	44.4	<2	<3	217		22.8			0.21	1.35		<0.05			
169	MSB-4	34.8	48.5	62.2	36.2	<2	<3	182		52.4			0.28	1.14		<0.05			
	MSB-4	15.8	20.75	25.7	48.2	<2	<3	218		14.0			0.21	1.62	0.14	0.11	<0.05		
	MSB-4	26.5	30.2	33.9	37.3	<2	<3	187		59.9			0.23	1.48	<0.05	3.52	<0.05		
	MSB-4	34.8	48.5	62.2	38.7	<2	<3	194		60.2			0.24	1.45	0.06	<0.05	<0.05		
	DH-15	63.0	67.75	72.5	25.8	2.4			2.52	11.9		<0.0004	0.8	0.8	<0.2	<0.3	<0.1	<0.7	<0.2
	DH-15	84.5	91	97.5	25.5	3.7			2.60	11.8		1.28	1.4	1.2	<0.2	<0.3	<0.1	<0.7	<0.2
TOKI LIGNITE BEARING F. (LOWER)																			
1	KNA-6 sed.	-			17.9		22.4	67.5		0.86	<0.05		4.55	1.02	<0.02	0.04			
2	KNA-6 unconf.	-			21.42		<1	107.1		0.05			4.29	0.87	<0.02	<0.02			
2	KNA-6 unconf.	-			20	<1	13.0	89.6		0.21			4.41	0.72	<0.02	<0.02	<0.02		
150	DH-12	157.5	160.79	164.1	7.36	4.82			1.10	<0.4		<0.1	14.8	53.3	<0.2	<0.3	<0.2		<0.2
159	MIU-4	71.5	74.11	76.8	17.9	1.5			1.76	4.94		<0.1	6.67	1.03	<0.1	<0.1	<0.1		<0.2
164	MSB-2	79.0	104.75	130.5	6.0	1.6			0.68	0.81		0.082	11	155	<0.2	<0.3	0.29	<0.5	<0.1
165	MSB-2	132.0	142.99	154.0	4.0	0.7			0.45	<0.4		0.042	8.3	223	<0.2	<0.3	0.42	<0.5	<0.1
TOKI GRANITE																			

Table A4-1 continued.

Index	Location	Depth			IC	TOC	CO_3^{2-} 1)	HCO_3^- 1)	alk.	SO_4^{2-}	HS^-	S^{2-}	F^-	Cl^-	NO_2^-	NO_3^-	Br^-	I^-	NH_4^+
		Min	Middle	Max															
		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	meq/l	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
3	KNA-6 gra.	-			23	1.1	<1	110.4		0.17	<0.05		3.78	1.06	<0.02	<0.02			<0.01
3	KNA-6 gra.	-			19.9	<1	5.3	96.3		0.11			3.73	0.63	<0.02	<0.02	<0.02		
170	DH-2	207.5	208.5	209.5	12.3	<2	<3	66.9		6.27			9.65	93.9		<0.05	0.18		
171	DH-2	228.5	232.75	237.0	10.8	<2	<3	56.7		3.60			8.79	106		<0.05	0.21		
172	DH-2	302.7	303.7	304.7	3.9	<2	4.52	33.2		3.89			9.85	145		<0.05	0.29		
173	DH-2	305.6	306.55	307.6	7.1	<2	6.59	30.9		3.91			9.18	138		<0.05	0.27		
174	DH-2	309.7	310.7	311.7	7.1	<2	5.07	33.0		3.90			9.46	146		<0.05	0.28		
175	DH-2	313.0	314	315.0	7.3	<2	3.83	35.3		3.74			9.07	150		<0.05	0.29		
176	DH-2	320.9	324.65	328.4	7.2	<2	<3	45.6		3.70			8.76	158		<0.05	0.28		
177	DH-2	347.8	348.8	349.8	5.5	<2	<3	34.9		3.96			8.05	191		<0.05	0.34		
178	DH-2	365.5	366.5	367.5	5.1	<2	5.14	23.6		3.74			7.78	211		<0.05	0.35		
179	DH-2	439.5	443.75	448.0	4.7	<2	4.9	21.9		3.22			6.52	228		<0.05	0.42		
180	DH-2	451.2	455.45	459.7	4.4	<2	2.9	24.5		2.26			6.12	267		<0.05	0.47		
	DH-7	438.0	441.25	444.5					0.73	5.6			0.75	4.31		<0.1			
	DH-7	479.0	482.25	485.5					0.89	6.8			2.38	4.47		<0.1			
	DH-7	479.0	482.25	485.5					0.83	5.73			3.81	3.87		<0.1			
108	DH-7	560.5	563.75	567.0	18	2.4			1.51	4.64		n.d.	2.11	4.37	0.01	0.01	n.d.		22.9
	DH-7	560.5	563.75	567.0					1.25	6.5			5.34	4.20		<0.1			
	DH-7	560.5	563.75	567.0					0.83	6.33			4.79	3.53		<0.1			
	DH-7	598.0	601.25	604.5					1.49	4.5			6.37	5.87		<0.1			

Table A4-1 continued.

Index	**Location**	**Depth**			**IC**	**TOC**	**CO_3^{2-} 1)**	**HCO_3^- 1)**	**alk.**	**SO_4^{2-}**	**HS^-**	**S^{2-}**	**F^-**	**Cl^-**	**NO_2^-**	**NO_3^-**	**Br^-**	**I^-**	**NH_4^+**
		Min	**Middle**	**Max**															
		mbgl	**mbgl**	**mbgl**	**ppm**	**ppm**	**ppm**	**ppm**	**meq/l**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	DH-7	598.0	601.25	604.5					1.26	4.19			7.11	5.67		<0.1			
	DH-7	660.0	663.25	666.5					0.97	5.0			4.42	4.20		<0.1			
	DH-7	660.0	663.25	666.5					1.01	4.57			7.79	2.84		0.20			
	DH-7	735.5	738.75	742.0					2.08	6.0			6.34	6.41		0.40			
	DH-7	735.5	738.75	742.0					1.96	2.78			8.67	6.10		<0.1			
109	DH-7	833.5	836.75	840.0	20	1.3			1.65	5.55		n.d.	9.95	3.09	0.1	0.05	n.d.		2.98
	DH-7	833.5	836.75	840.0					1.48	4.2			9.24	4.31		<0.1			
110	DH-7	880.0	883.25	886.5	22	2.8			1.79	5.35		n.d.	8.62	5.08	0.09	0.03	n.d.		4.56
	DH-7	880.0	883.25	886.5					1.63	2.8			10.2	6.48		<0.1			
	DH-7	880.0	883.25	886.5					1.55	1.96			10.2	5.80		<0.1			
151	DH-12	171.8	225.99	280.2	6.41	<1			0.68	<0.4		<0.1	12.5	52.6	<0.2	<0.3	<0.2		<0.2
155	DH-12	431.4	451.96	472.5	5.39	<1			0.64	<0.4		<0.1	12.8	72.1	<0.2	<0.3	<0.2		<0.2
156	DH-12	388.9	409.29	429.7	3.13	1.2			0.37	<0.4		<0.1	9.40	175	<0.2	<0.3	0.37		<0.2
157	DH-12	345.9	366.54	387.2	3.82	<1			0.44	<0.4		<0.1	9.79	137	<0.2	<0.3	0.32		<0.2
158	DH-12	279.4	312.04	344.7	4.90	<1			0.52	<0.4		<0.1	10.0	99.9	<0.2	<0.3	<0.2		<0.2
160	MIU-4	82.3	99.37	116.5	18	0.8			1.54	3.14		0.05	11.05	0.86	<0.1	<0.1	<0.1		<0.2
161	MIU-4	272.8	273.62	274.5	16	1.4			1.44	<0.3		<0.1	11.95	1.07	<0.1	<0.1	<0.1		<0.2
162	MIU-4	505.8	533.09	560.4	16	1.7			1.40	<0.3		<0.1	12.93	1.23	<0.1	<0.1	<0.1		<0.2
163	MIU-4	653.4	668.84	684.3	17.0	2.7			1.55	<0.3		<0.1	11.88	1.19	<0.1	<0.1	<0.1		<0.2
166	MSB-2	171.5	173.49	175.5	5.4	0.6			0.56	1.6		0.048	8.0	189	<0.2	<0.3	0.25	<0.5	<0.1

Table A4-1 continued.

Index	Location	Depth			IC	TOC	CO_3^{2-} 1)	HCO_3^- 1)	alk.	SO_4^{2-}	HS^-	S^{2-}	F^-	Cl^-	NO_2^-	NO_3^-	Br^-	I^-	NH_4^+
		Min	**Middle**	**Max**															
		mbgl	**mbgl**	**mbgl**	**ppm**	**ppm**	**ppm**	**ppm**	**meq/l**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
167	MSB-4	95.5	97.25	99.0	8.9	1.1			0.77	<0.4		0.5	12	96	<0.2	<0.3	0.18	<0.5	<0.1
	MIZ-1	113.1	114.67	116.3	9.6	<1			1.27	6.8		0.09	8.7	38	<0.2	<0.3	<0.1	<0.7	<0.2
	MIZ-1	215.0	220.34	225.7	6.6	2.8			0.68	8.4		4.49	11.9	85	<0.2	<0.3	0.2	<0.7	<0.2
Units		mabh	mabh	mabh	mg/l	mg/l	mg/l	mg/l	$[meq/l^{-1}]$	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l
TOKI GRANITE																			
	MIZ-1	580.80	588.95	597.10	5.9	1.8			0.56	1.2		0.04	8.0	179.4	<0.2	<0.3	<0.1	<0.7	<0.2
	MIZ-1	649.00	687.48	725.96	3.7	3.0			0.39	0.9		0.02	6.4	243.9	<0.2	<0.3	0.4	<0.7	<0.2
TOKI LIGNITE BEARING F. (LOWER)																			
	DH-15	102.70	118.2	133.70	8.3	2.4			1.74	5.6		1.88	12.5	22.2	<0.2	<0.3	<0.1	<0.7	<0.2
	DH-15	152.10	184.27	216.43	8.6	1			1.04	1.1		4.45	10.9	52.5	<0.2	<0.3	<0.1	<0.7	<0.2
TOKI GRANITE																			
	DH-15	233.55	236.78	240.00	4	2			0.61	<0.4		7.04	8.3	173.5	<0.2	<0.3	0.4	<0.7	<0.2
	DH-15	437.60	449.85	462.1	5.8	1.9			0.57	1.1		0.51	6.8	186.7	<0.2	<0.3	0.5	<0.7	<0.2
	DH-15	575.50	587.75	600.00	3.4	2.5			0.36	1.3		0.04	5.3	383.4	<0.2	<0.3	0.9	<0.7	<0.2
	DH-15	765.00	773.25	781.5	1.6	3.2			0.19	<0.4		0.17	3.7	768.8	<0.2	<0.3	1.3	<0.7	<0.2

Table A4-1 continued.

Index	Location	Depth			IC	TOC	CO_3^{2-} 1)	HCO_3^- 1)	alk.	SO_4^{2-}	HS^-	S^{2-}	F^-	Cl^-	NO_2^-	NO_3^-	Br^-	I^-	NH_4^+
		Min	Middle	Max															
		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	meq/l	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm	ppm
	DH-15	937.00	945.25	953.50	3.3	2.8			0.32	<0.4		0.81	2.8	843.3	<0.2	<0.3	1.6	<0.7	<0.2
	DH-15	987.00	995.25	1003.5	0.9	4.1			0.16	<0.4		0.61	1.7	1614	<0.2	<0.3	2.9	<0.7	<0.2

Table A4-1 continued.

Index	Location	Depth			PO_4^{3-}	Si	Al	ΣFe	Fe^{2+}	Fe^{3+}	ΣMn	B	U	δD	$\delta^{18}O$	$\delta^{13}C$	C-14 activity	C-14 age
		Min	Middle	Max														
Units		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	ppm	ppm	ppm			‰SMOW	‰SMOW	‰	% MC	yB.P.
AKEYO F.																		
168	MSB-4	15.8	20.75	25.7		33.7		<0.01			0.51							
169	MSB-4	34.8	48.5	62.2		30.9		<0.01			0.22							
	MSB-4	15.8	20.75	25.7	0.18	33.9	<0.2	<0.01	<0.05	<0.01	0.48			-50.3	-7.5	-19.5	91.9	
	MSB-4	26.5	30.2	33.9	0.05	31.4	<0.2	<0.01	<0.05	<0.01	0.29			-55.8	-8.2	-18.6	55.2	
	MSB-4	34.8	48.5	62.2	0.10	32.5	<0.2	<0.01	<0.05	<0.01	0.24			-55.8	-8.2	-19.6	48.4	
	DH-15	63.0	67.75	72.5		34.6	0.023	0.061			0.004			-57.9	-8.4			
	DH-15	84.5	91	97.5		21.5	0.21	0.25			0.006			-58.3	-8.5			
TOKI LIGNITE BEARING F. (LOWER)																		
1	KNA-6 sed.	-			<0.02	7.41	<0.1	0.04	<0.05	<0.05	<0.01			-59.4	-9.0			
2	KNA-6 unconf.	-			<0.02	7.51	<0.1	<0.02	<0.05	<0.05	<0.01			-57.7	-8.5		22.1	
2	KNA-6 unconf.	-			<0.02	8.09	<0.1	<0.02			<0.01							
150	DH-12	157.5	160.79	164.1		7.02	<0.1	<0.05	<0.05		<0.005			-59.1	-9.0	-5.0	11.0	
159	MIU-4	71.5	74.11	76.8		5.8	<0.1	<0.05	<0.05		<0.005			-54.3	-8.6	-18.9	28.3	
164	MSB-2	79.0	104.75	130.5		4.9	0.012	0.019	<0.05		0.0062			-57.8	-9.1	-13.4	57.8	
165	MSB-2	132.0	142.99	154.0		5.7	0.014	0.017	<0.05		0.02			-57.0	-9.1	-12.4	48.4	
TOKI GRANITE			0															

Table A4-1 continued.

Index	Location	Depth			PO_4^{3-}	Si	Al	ΣFe	Fe^{2+}	Fe^{3+}	ΣMn	B	U	δD	$\delta^{18}O$	$\delta^{13}C$	C-14 activity	C-14 age
		Min	Middle	Max														
		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	ppm	ppm	ppm			‰SMOW	‰SMOW	‰	% MC	yB.P.
3	KNA-6 gra.	-			<0.02	10.73	<0.1	<0.02	<0.05	<0.05	<0.01			-59.2	-8.7	-17.3	22.0	
3	KNA-6 gra.	-			<0.02	10.88	<0.1	<0.02			0.01							
170	DH-2	207.5	208.5	209.5		6.94		0.02			0.02			-60.4	-9.0			
171	DH-2	228.5	232.75	237.0		6.85		<0.01			<0.01			-60.0	-8.9			
172	DH-2	302.7	303.7	304.7		6.61		<0.01			<0.01							
173	DH-2	305.6	306.55	307.6		6.04		0.03			<0.01							
174	DH-2	309.7	310.7	311.7		6.69		0.01			<0.01			-60.3	-8.9			
175	DH-2	313.0	314	315.0		6.59		0.02			<0.01							
176	DH-2	320.9	324.65	328.4		6.24		<0.01			<0.01							
177	DH-2	347.8	348.8	349.8		6.77		0.03			<0.01							
178	DH-2	365.5	366.5	367.5		6.42		<0.01			<0.01			-59.4	-8.9			
179	DH-2	439.5	443.75	448.0		6.50		<0.01			<0.01			-60.8	-9.0	-10.8	27.3	
180	DH-2	451.2	455.45	459.7		6.38		<0.01			<0.01			-60.5	-9.0			
	DH-7	438.0	441.25	444.5		4.5		<0.01										
	DH-7	479.0	482.25	485.5		9.7		<0.01										
	DH-7	479.0	482.25	485.5		13.0		<0.05										
108	DH-7	560.5	563.75	567.0	0.086	1.9	0.19	8.9	8.5		0.16			-53.0	-8.0	-16.9	50.6	5480
	DH-7	560.5	563.75	567.0		24.3		<0.01										
	DH-7	560.5	563.75	567.0		20.1		<0.1										
	DH-7	598.0	601.25	604.5		22.3		0.04										

Table A4-1 continued.

Index	Location	Depth			PO_4^{3-}	Si	Al	ΣFe	Fe^{2+}	Fe^{3+}	ΣMn	B	U	δD	$\delta^{18}O$	$\delta^{13}C$	C-14 activity	C-14 age
		Min	Middle	Max														
		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	ppm	ppm	ppm			‰SMOW	‰SMOW	‰	% MC	yB.P.
	DH-7	598.0	601.25	604.5		20.8		<0.05										
	DH-7	660.0	663.25	666.5		12.6		0.01										
	DH-7	660.0	663.25	666.5		13.2		<0.1										
	DH-7	735.5	738.75	742.0		27.7		0.03										
	DH-7	735.5	738.75	742.0		27.6		<0.1										
109	DH-7	833.5	836.75	840.0	0.039	8.5	1.2	7.2	6.9		0.10			-58.0	-8.5	-15.9	22.5	12000
	DH-7	833.5	836.75	840.0		17.1		0.02										
110	DH-7	880.0	883.25	886.5	0.328	14.7	4.3	7.5	8.8		0.31			-54.0	-8.2	-15.5	39.0	7570
	DH-7	880.0	883.25	886.5		29.8		0.87										
	DH-7	880.0	883.25	886.5		22.4		0.6										
151	DH-12	171.8	225.99	280.2		6.85	<0.1	<0.05	<0.05		<0.005			-56.7	-8.8	-15.4	10.8	
155	DH-12	431.4	451.96	472.5		6.48	<0.1	<0.05	<0.05		<0.005			-56.9	-9.0			
156	DH-12	388.9	409.29	429.7		6.68	<0.1	<0.05	<0.05		<0.005			-56.5	-8.8			
157	DH-12	345.9	366.54	387.2		7.32	<0.1	<0.05	<0.05		<0.005			-56.1	-8.9			
158	DH-12	279.4	312.04	344.7		6.66	<0.1	<0.05	<0.05		<0.005			-56.6	-8.7			
160	MIU-4	82.3	99.37	116.5		5.9	<0.1	0.07	<0.05		<0.005			-53.3	-8.5	-18.6	20.7	
161	MIU-4	272.8	273.62	274.5		6.2	<0.1	0.06	<0.05		<0.005			-53.9	-8.6			
162	MIU-4	505.8	533.09	560.4		7.3	<0.1	<0.05	<0.05							-17.7	22.2	
163	MIU-4	653.4	668.84	684.3		8.1	<0.1	<0.05	<0.05		<0.005			-55.2	-8.8	-16.1	12.7	
166	MSB-2	171.5	173.49	175.5		5.5	0.004	0.058	<0.05		0.02			-61.0	-8.9	-13.2	33.1	

Table A4-1 continued.

Index	Location	Depth			PO_4^{3-}	Si	Al	ΣFe	Fe^{2+}	Fe^{3+}	ΣMn	B	U	δD	$\delta^{18}O$	$\delta^{13}C$	C-14 activity	C-14 age
		Min	Middle	Max														
		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	ppm	ppm	ppm			‰SMOW	‰SMOW	‰	% MC	yB.P.
167	MSB-4	95.5	97.25	99.0		6.1	0.069	0.042	<0.05		0.005			-61.8	-8.9	-14.3	15.0	
	MIZ-1	113.1	114.67	116.3		8.6	0.058	0.021	<0.05		0.0018			-60.7	-8.8			
	MIZ-1	215.0	220.34	225.7		4.5	0.889	0.086	<0.05		0.084			-59.6	-8.8			
Units		mabh	mabh	mabh		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	[‰]	[‰]	[‰]	[pMC]	yB.P.
TOKI GRANITE																		
	MIZ-1	580.80	588.95	597.10		6.5	0.006	0.039	<0.05		0.017	1.22	0.0008	-61.1	-8.9	-14.1	34.83±0.28	
	MIZ-1	649.00	687.48	725.96		6.3	0.048	0.006	<0.05		0.007	2.07	0.00024	-58.2	-8.9	-12.1	41.92±0.53	
TOKI LIGNITE BEARING F. (LOWER)																		
	DH-15	102.70	118.2	133.70		12.1	0.48	0.29	0.11		0.006	1.76	0.00021	-61.2	-8.7			
	DH-15	152.10	184.27	216.43		7.2	0.1	0.055	<0.05		0.001	0.6	0.00009	-61.4	-9			
TOKI GRANITE																		
	DH-15	233.55	236.78	240.00		8.1	0.1	0.08	<0.05		0.003	1.26	0.00012	-60.5	-9			
	DH-15	437.60	449.85	462.1		6	0.048	0.006	<0.05		0.007	1.2	0.00043	-58.7	-8.7			
	DH-15	575.50	587.75	600.00		6.9	0.035	0.022	<0.05		0.011	1.49	0.00037	-60.1	-8.9			
	DH-15	765.00	773.25	781.5		7.4	0.022	0.012	<0.05		0.037	2.09	0.00017	-58.5	-8.8			

Table A4-1 continued.

Index	Location	Depth			PO_4^{3-}	Si	Al	ΣFe	Fe^{2+}	Fe^{3+}	ΣMn	B	U	δD	$\delta^{18}O$	$\delta^{13}C$	C-14 activity	C-14 age
		Min	Middle	Max														
		mbgl	mbgl	mbgl	ppm	ppm	ppm	ppm	ppm	ppm	ppm			‰SMOW	‰SMOW	‰	% MC	yB.P.
	DH-15	937.00	945.25	953.50		7.5	0.016	0.023	<0.05		0.165	1.67	0.0032	-57.4	-8.5			
	DH-15	987.00	995.25	1003.5		8.1	0.028	0.021	<0.05		0.038	2.42	0.00005	-57.4	-8.7			

Table A4-1 continued.

index	location	Depth			^{14}C/^{12}C	Tritium	^{234}U/^{238}U	^{234}U/^{238}U	^{228}Th	^{230}Th	Rn	δ^{34}S	^{36}Cl/Cl	Note
		Min	Middle	Max										
Units		mbgl	mbgl	mbgl	[pMC]	T.U.	activity ratio	activity ratio	mBq/l	mBq/l	Bq/l	‰		
AKEYO F.														
168	MSB-4	15.8	20.75	25.7		0.6								
169	MSB-4	34.8	48.5	62.2		0.6								
	MSB-4	15.8	20.75	25.7										
	MSB-4	26.5	30.2	33.9										
	MSB-4	34.8	48.5	62.2										
	DH-15	63.0	67.75	72.5		0.4								
	DH-15	84.5	91	97.5		<0.3								
TOKI LIGNITE BEARING F. (LOWER)														
1	KNA-6 sed.	-				<0.3								Test interval was 32.05 - 33.05mabh.
2	KNA-6 unconf.	-				<0.3								Test interval was 43.50 - 46.00mabh.
2	KNA-6 unconf.	-												Test interval was 43.50 - 46.00mabh.
150	DH-12	157.5	160.79	164.1		<0.31								
159	MIU-4	71.5	74.11	76.8		<1.0								
164	MSB-2	79.0	104.75	130.5		<0.46	3.3±0.23	-	-	0.065±0.014		-		Hydrogen sulphide bubble
165	MSB-2	132.0	142.99	154.0		<0.42	5.7±0.19	0.036±0.0049	0.14±0.027	0.075±0.018		-		Hydrogen sulphide bubble

Table A4-1 continued.

Index	Location	Depth			$^{14}C/^{12}C$	Tritium	$^{234}U/^{238}U$	$^{234}U/^{238}U$	^{228}Th	^{230}Th	Rn	$\delta^{34}S$	$^{36}Cl/Cl$	Note
		Min	Middle	Max										
		mbgl	mbgl	mbgl	[pMC]	T.U.	activity ratio	activity ratio	mBq/l	mBq/l	Bq/l	‰		
TOKI GRANITE														
3	KNA-6 gra.	-				<0.3								Test interval was 50.50 - 101.00mabh.
3	KNA-6 gra.	-												Test interval was 50.50 - 101.00mabh.
170	DH-2	207.5	208.5	209.5		1.5								Drilling fluid was without any tracer.
171	DH-2	228.5	232.75	237.0		1.3								Drilling fluid was without any tracer.
172	DH-2	302.7	303.7	304.7										Drilling fluid was without any tracer.
173	DH-2	305.6	306.55	307.6										Drilling fluid was without any tracer.
174	DH-2	309.7	310.7	311.7		0.93								Drilling fluid was without any tracer.
175	DH-2	313.0	314	315.0										Drilling fluid was without any tracer.
176	DH-2	320.9	324.65	328.4										Drilling fluid was without any tracer.
177	DH-2	347.8	348.8	349.8										Drilling fluid was without any tracer.
178	DH-2	365.5	366.5	367.5		1.0								Drilling fluid was without any tracer.
179	DH-2	439.5	443.75	448.0		<0.54								Drilling fluid was without any tracer.
180	DH-2	451.2	455.45	459.7		0.77								Drilling fluid was without any tracer.
	DH-7	438.0	441.25	444.5		2.2								
	DH-7	479.0	482.25	485.5		4.5								
	DH-7	479.0	482.25	485.5		1.4								
108	DH-7	560.5	563.75	567.0		2.3								

Table A4-1 continued.

Index	Location	Depth			$^{14}C/^{12}C$	Tritium	$^{234}U/^{238}U$	$^{234}U/^{238}U$	^{228}Th	^{230}Th	Rn	$\delta^{34}S$	$^{36}Cl/Cl$	Note
		Min	Middle	Max										
		mbgl	mbgl	mbgl	[pMC]	T.U.	activity ratio	activity ratio	mBq/l	mBq/l	Bq/l	‰		
	DH-7	560.5	563.75	567.0		2.1								
	DH-7	560.5	563.75	567.0		1.0								
	DH-7	598.0	601.25	604.5		<0.9								
	DH-7	598.0	601.25	604.5		1.0								
	DH-7	660.0	663.25	666.5		4.0								
	DH-7	660.0	663.25	666.5		<0.5								
	DH-7	735.5	738.75	742.0		4.7								
	DH-7	735.5	738.75	742.0		1.2								
109	DH-7	833.5	836.75	840.0		3.4								
	DH-7	833.5	836.75	840.0		4.3								
110	DH-7	880.0	883.25	886.5		2.1								
	DH-7	880.0	883.25	886.5		6.8								
	DH-7	880.0	883.25	886.5		0.9								
151	DH-12	171.8	225.99	280.2		<0.28								
155	DH-12	431.4	451.96	472.5		<0.29								
156	DH-12	388.9	409.29	429.7		<0.31								
157	DH-12	345.9	366.54	387.2		<0.3								
158	DH-12	279.4	312.04	344.7		<0.31								
160	MIU-4	82.3	99.37	116.5		<0.30								
161	MIU-4	272.8	273.62	274.5		<0.30								

Table A4-1 continued.

Index	Location	Depth			$^{14}C/^{12}C$	Tritium	$^{234}U/^{238}U$	$^{234}U/^{238}U$	^{228}Th	^{230}Th	Rn	$\delta^{34}S$	$^{36}Cl/Cl$	Note
		Min	Middle	Max										
		mbgl	mbgl	mbgl	[pMC]	T.U.	activity ratio	activity ratio	mBq/l	mBq/l	Bq/l	‰		
162	MIU-4	505.8	533.09	560.4										
163	MIU-4	653.4	668.84	684.3		<0.33								Sodium naphthionate (tracer): 0.14ppm
166	MSB-2	171.5	173.49	175.5		<0.44	5.0±0.18	0.033±0.0037	0.26±0.029	0.098±0.017				weathered zone
167	MSB-4	95.5	97.25	99.0		<0.41	4.2±0.23	0.042±0.013	0.051±0.016	0.058±0.015				
	MIZ-1	113.1	114.67	116.3		<0.3								
	MIZ-1	215.0	220.34	225.7		0.3								
Units		mabh	mabh	mabh	[pMC]	[TU]								
TOKI GRANITE														
	MIZ-1	580.80	588.95	597.10	34.96±0.28	<0.30								
	MIZ-1	649.00	687.48	725.96	41.84±0.53	<0.29								
TOKI LIGNITE BEARING F. (LOWER)														
	DH-15	102.70	118.2	133.70		<0.3							-	
	DH-15	152.10	184.27	216.43		0.4							69±12	
TOKI GRANITE														
	DH-15	233.55	236.78	240.00		<0.3							39±12	

Table A4-1 continued.

Index	**Location**	**Depth**			**$^{14}C/^{12}C$**	**Tritium**	**$^{234}U/^{238}U$**	**$^{234}U/^{238}U$**	**^{228}Th**	**^{230}Th**	**Rn**	**$\delta^{34}S$**	**$^{36}Cl/Cl$**	**Note**
		Min	**Middle**	**Max**										
		mbgl	**mbgl**	**mbgl**	**[pMC]**	**T.U.**	**activity ratio**	**activity ratio**	**mBq/l**	**mBq/l**	**Bq/l**	**‰**		
	DH-15	437.60	449.85	462.1		0.48								
	DH-15	575.50	587.75	600.00		<0.32								
	DH-15	765.00	773.25	781.5		<0.32								
	DH-15	937.00	945.25	953.50		0.33								
	DH-15	987.00	995.25	1003.5										

Table A4-2 Quality indicators used during the development of the quality classification methodology.

Index	Location	Depth			During sampling				During analysis			
		Min	Middle	Max	Smell	Colour change	Gas bubbles	Precipitation	Smell	Colour change	Gas bubbles	Precipitation
Units		mbgl	mbgl	mbgl								
AKEYO F.												
168	MSB-4	15.8	20.75	25.7								
169	MSB-4	34.8	48.5	62.2								
	MSB-4	15.8	20.75	25.7								
	MSB-4	26.5	30.2	33.9								
	MSB-4	34.8	48.5	62.2								
	DH-15	63.0	67.75	72.5								
	DH-15	84.5	91	97.5								
TOKI LIGNITE BEARING F. (LOWER)												
1	KNA-6 sed.	-										
2	KNA-6 unconf.	-										
2	KNA-6 unconf.	-										
150	DH-12	157.5	160.79	164.1								
159	MIU-4	71.5	74.11	76.8	No	No	No	No	No	No	No	No
164	MSB-2	79.0	104.75	130.5	A little	No	Yes	No	A little	No	No	No
165	MSB-2	132.0	142.99	154.0	A little	No	Yes	No	A little	No	No	No
TOKI GRANITE			0									
3	KNA-6 gra.	-										
3	KNA-6 gra.	-										

Table A4-2 continued.

Index	Location	Depth			During sampling				During analysis			
		Min	Middle	Max	Smell	Colour change	Gas bubbles	Precipitation	Smell	Colour change	Gas bubbles	Precipitation
		mbgl	mbgl	mbgl								
170	DH-2	207.5	208.5	209.5								
171	DH-2	228.5	232.75	237.0								
172	DH-2	302.7	303.7	304.7								
173	DH-2	305.6	306.55	307.6								
174	DH-2	309.7	310.7	311.7								
175	DH-2	313.0	314	315.0								
176	DH-2	320.9	324.65	328.4								
177	DH-2	347.8	348.8	349.8								
178	DH-2	365.5	366.5	367.5								
179	DH-2	439.5	443.75	448.0								
180	DH-2	451.2	455.45	459.7								
	DH-7	438.0	441.25	444.5								
	DH-7	479.0	482.25	485.5								
	DH-7	479.0	482.25	485.5								
108	DH-7	560.5	563.75	567.0								
	DH-7	560.5	563.75	567.0								

Table A4-2 continued.

Index	Location	Depth			During sampling				During analysis			
		Min	Middle	Max	Smell	Colour change	Gas bubbles	Precipitation	Smell	Colour change	Gas bubbles	Precipitation
		mbgl	mbgl	mbgl								
	DH-7	560.5	563.75	567.0								
	DH-7	598.0	601.25	604.5								
	DH-7	598.0	601.25	604.5								
	DH-7	660.0	663.25	666.5								
	DH-7	660.0	663.25	666.5								
	DH-7	735.5	738.75	742.0								
	DH-7	735.5	738.75	742.0								
109	DH-7	833.5	836.75	840.0								
	DH-7	833.5	836.75	840.0								
110	DH-7	880.0	883.25	886.5								
	DH-7	880.0	883.25	886.5								
	DH-7	880.0	883.25	886.5								
151	DH-12	171.8	225.99	280.2								
155	DH-12	431.4	451.96	472.5								
156	DH-12	388.9	409.29	429.7								
157	DH-12	345.9	366.54	387.2								
158	DH-12	279.4	312.04	344.7								
160	MIU-4	82.3	99.37	116.5	No	No	No	White suspended matter	No	No	No	No
161	MIU-4	272.8	273.62	274.5	No	No	No	White suspended matter	No	No	No	No

Table A4-2 continued.

Index	Location	Depth			During sampling				During analysis			
		Min	**Middle**	**Max**	**Smell**	**Colour change**	**Gas bubbles**	**Precipitation**	**Smell**	**Colour change**	**Gas bubbles**	**Precipitation**
		mbgl	**mbgl**	**mbgl**								
162	MIU-4	505.8	533.09	560.4	No	No	No	No	No	No	No	No
163	MIU-4	653.4	668.84	684.3	No	No	No	No	No	No	No	No
166	MSB-2	171.5	173.49	175.5	A little	No	Yes	No	A little	No	No	No
167	MSB-4	95.5	97.25	99.0	A little	No	Yes	No	Strong	No	No	No
	MIZ-1	113.1	114.67	116.3	Hydrogen sulfide	No	No	No	Hydrogen sulfide	No	No	No
	MIZ-1	215.0	220.34	225.7	Hydrogen sulfide	No	Yes	No	Hydrogen sulfide	No	No	No
Units		mabh	mabh	mabh								
TOKI GRANITE												
	MIZ-1	580.80	588.95	597.10	Weak hydrogen sulfide	Light yellow-green	Yes	No	Weak hydrogen sulfide	Light yellow-green	No	No
	MIZ-1	649.00	687.48	725.96	No	Light yellow-green	Yes	No	No	Light yellow-green	No	No
TOKI LIGNITE BEARING F. (LOWER)												
	DH-15	102.70	118.2	133.70	Weak	No	No	No	Weak	No	No	No
	DH-15	152.10	184.27	216.43	Strong	No	Yes	No	Strong	No	Yes	No
TOKI GRANITE												
	DH-15	233.55	236.78	240.00	Strong	No	Yes	No	Strong	No	Yes	No
	DH-15	437.60	449.85	462.1	Weak	Light pink	Yes	No	Weak	Light pink	Yes	No

Table A4-2 continued.

Index	Location	Depth			During sampling				During analysis			
		Min	Middle	Max	Smell	Colour change	Gas bubbles	Precipitation	Smell	Colour change	Gas bubbles	Precipitation
		mbgl	mbgl	mbgl								
	DH-15	575.50	587.75	600.00	Weak	Light pink	Yes	No	Weak	Light pink	Yes	No
	DH-15	765.00	773.25	781.5	Weak	Light pink	No	No	Weak	Light pink	No	No
	DH-15	937.00	945.25	953.50	Weak	No	Yes	No	Weak	No	Yes	No
	DH-15	987.00	995.25	1003.5	Weak	No	Yes	No	Weak	No	No	No

Table A4-2 continued.

Index	Location	Depth			Drilling fluid tracers			Drilling fluid contamination	Charge balance	Sample container	Stability of pH	Stability of EC	Stability of Eh	Distance between packers	Sampling location
		Min	Middle	Max	Uranine Tracer	Amino-G acid	Eosin	%	%		/hour	mS/m/hour	mV/hour	m	
Units		mbgl	mbgl	mbgl											
AKEYO F.															
168	MSB-4	15.8	20.75	25.7				0.200	5.29	2				9.9	2
169	MSB-4	34.8	48.5	62.2				0.100	4.24	2				27.4	2
	MSB-4	15.8	20.75	25.7				0.400	-1.48	2				9.9	2
	MSB-4	26.5	30.2	33.9				0.100	-4.74	2				7.4	2
	MSB-4	34.8	48.5	62.2				0.300	-2.50	2				27.4	2
	DH-15	63.0	67.75	72.5				0.5	2.62	2	-0.004	0.02	-2.4	9.5	2
	DH-15	84.5	91	97.5				2.1	4.46	2	0.001	0.01	1.8	13	2
TOKI LIGNITE BEARING F. (LOWER)															
1	KNA-6 sed.	-						0.1	-0.82	2				0.7071	2
2	KNA-6 unconf.	-						0.1	-6.48	2				1.7678	2
2	KNA-6 unconf.	-						0.1	-3.22	2				1.7678	2
150	DH-12	157.5	160.79	164.1				0.68	1.03	2	-0.02	0.01	-4.6	6.67	2
159	MIU-4	71.5	74.11	76.8				0.6	0.70	2	0.001	0.01	-2	5.32	2
164	MSB-2	79.0	104.75	130.5				1.7	-1.12	2	0.001	0.01	-0.6	51.49	2
165	MSB-2	132.0	142.99	154.0				1.8	-0.37	2	-0.006	-0.02	-1.2	22	2

🟨	Calculated for this study by R. Metcalfe
🟦	From Arthur, R.C. 2003. Empirical constraints on theoretical models of the chemical evolution of groundwaters in the Tono area. Monitor Scientific Draft Final Report

Sample container: 1 = downhole sampling vessel that maintains in-situ conditions; 2 = polythene bottle used to collect samples at the surface

Sampling location: 1 = downhole (1000 m sampling device, MP system etc); 2 = Sampled at the surface during a hydraulic test

Table A4-2 continued.

Index	Location	Depth			Drilling fluid tracers			Drilling fluid contamination	Charge balance	Sample container	Stability of pH	Stability of EC	Stability of Eh	Distance between packers	Sampling location
		Min	Middle	Max	Uranine Tracer	Amino-G acid	Eosin	%	%		/hour	mS/m/hour	mV/hour	m	
		mbgl	mbgl	mbgl											
TOKI GRANITE															
3	KNA-6 gra.	-						0.1	-6.81	2				35.709	2
3	KNA-6 gra.	-						0.1	1.63	2				35.709	2
170	DH-2	207.5	208.5	209.5					-2.90	2				2	2
171	DH-2	228.5	232.75	237.0					8.00	2				8.5	2
172	DH-2	302.7	303.7	304.7					2.26	2				2	2
173	DH-2	305.6	306.55	307.6					-4.07	2				2	2
174	DH-2	309.7	310.7	311.7					-2.51	2				2	2
175	DH-2	313.0	314	315.0					-1.07	2				2	2
176	DH-2	320.9	324.65	328.4					-1.16	2				7.5	2
177	DH-2	347.8	348.8	349.8					-0.11	2				2	2
178	DH-2	365.5	366.5	367.5					-5.13	2				2	2
179	DH-2	439.5	443.75	448.0					4.56	2				8.5	2
180	DH-2	451.2	455.45	459.7					3.81	2				8.5	2
	DH-7	438.0	441.25	444.5					0.87	2				6.5	1
	DH-7	479.0	482.25	485.5					2.56	2				6.5	1
	DH-7	479.0	482.25	485.5					3.02	2				6.5	1

Table A4-2 continued.

Index	Location	Depth			Drilling fluid tracers			Drilling fluid contamination	Charge balance	Sample container	Stability of pH	Stability of EC	Stability of Eh	Distance between packers	Sampling location
		Min	Middle	Max	Uranine Tracer	Amino-G acid	Eosin	%	%		/hour	mS/m/hour	mV/hour	m	
		mbgl	mbgl	mbgl											
108	DH-7	560.5	563.75	567.0					-22.6	1	0.001	0.01	-0.4	6.5	1
	DH-7	560.5	563.75	567.0					-4.87	2				6.5	1
	DH-7	560.5	563.75	567.0					4.03	2				6.5	1
	DH-7	598.0	601.25	604.5					4.66	2				6.5	1
	DH-7	598.0	601.25	604.5						2				6.5	1
	DH-7	660.0	663.25	666.5					4.47	2				6.5	1
	DH-7	660.0	663.25	666.5						2				6.5	1
	DH-7	735.5	738.75	742.0						2				6.5	1
	DH-7	735.5	738.75	742.0						2				6.5	1
109	DH-7	833.5	836.75	840.0					-20.87	1	0.002	0.01	-0.8	6.5	1
	DH-7	833.5	836.75	840.0					21.06	2				6.5	1
110	DH-7	880.0	883.25	886.5					1.21	1	0.001	-0.06	-1.4	6.5	1
	DH-7	880.0	883.25	886.5					4.41	2				6.5	1
	DH-7	880.0	883.25	886.5					9.19	2				6.5	1
151	DH-12	171.8	225.99	280.2				0.04	-1.40	2	0.00	0.01	-0.6	108.37	2
155	DH-12	431.4	451.96	472.5				0.01	1.4	2	0.018	-0.02	-0.2	41.08	2
156	DH-12	388.9	409.29	429.7				2.00	0.18	2	0.001	-0.04	2	40.78	2
157	DH-12	345.9	366.54	387.2				2.58	1.00	2	-0.012	0.01	-0.4	41.28	2
158	DH-12	279.4	312.04	344.7				0.06	-0.78	2	0.01	0.28	-0.6	65.27	2

Table A4-2 continued.

Index	Location	Depth			Drilling fluid tracers			Drilling fluid contamination	Charge balance	Sample container	Stability of pH	Stability of EC	Stability of Eh	Distance between packers	Sampling location
		Min	**Middle**	**Max**	**Uranine Tracer**	**Amino-G acid**	**Eosin**	**%**	**%**		**/hour**	**mS/m/hour**	**mV/hour**	**m**	
		mbgl	**mbgl**	**mbgl**											
160	MIU-4	82.3	99.37	116.5				1.00	-2.89	2	0.06	0.01	0.7	34.16	2
161	MIU-4	272.8	273.62	274.5				2.67	-1.83	2	0.004	0.01	-4.4	1.74	2
162	MIU-4	505.8	533.09	560.4				2.67	-0.05	2	0.002	0.01	0.6	54.65	2
163	MIU-4	653.4	668.84	684.3				1.40	1.33	2	0.001	0.01	0.6	30.83	2
166	MSB-2	171.5	173.49	175.5				2.25	-0.71	2	0.001	-0.12	-1	4	2
167	MSB-4	95.5	97.25	99.0				0.35	-2.78	2	0.002	-0.04	-2.4	3.5	2
	MIZ-1	113.1	114.67	116.3				0.70	5.19	2	0.002	0.1	1.2	3.23	2
	MIZ-1	215.0	220.34	225.7				2.91	-5.74	2	0.02	0.04	9	10.67	2
Units		mabh	mabh	mabh											
TOKI GRANITE					mg/l	mg/l	mg/l								
	MIZ-1	580.80	588.95	597.10	0.0413	<0.005		20.65	-0.54	2				16.3	2
	MIZ-1	649.00	687.48	725.96	0.0702	<0.005		35.10	0.07	2				77.0	2
TOKI LIGNITE BEARING F. (LOWER)															2
	DH-15	102.70	118.2	133.70			0.133	13.30	6.16	2				31.0	2
	DH-15	152.10	184.27	216.43			0.029	2.90	2.96	2				64.3	2
TOKI GRANITE															2
	DH-15	233.55	236.78	240.00			0.01	1.00	6.35	2				6.4	2

Table A4-2 continued.

Index	Location	Depth			Drilling fluid tracers			Drilling fluid contamination	Charge balance	Sample container	Stability of pH	Stability of EC	Stability of Eh	Distance between packers	Sampling location
		Min	Middle	Max	Uranine Tracer	Amino-G acid	Eosin	%	%		/hour	mS/m/hour	mV/hour	m	
		mbgl	mbgl	mbgl											
	DH-15	437.60	449.85	462.1			0.338	33.80	1.96	2				24.5	2
	DH-15	575.50	587.75	600.00			0.166	16.60	1.41	2				24.5	2
	DH-15	765.00	773.25	781.5			0.1	12.80	-0.42	2				16.5	2
	DH-15	937.00	945.25	953.50			0.3	25.50	2.95	2				16.5	2
	DH-15	987.00	995.25	1003.5			0.032	3.21	2.62	2				16.5	2

Table A4-2 continued.

Index	Location	Depth			Physico-chemical parameter measuring location	Pumping rate	Total extracted water volume	DO	log f $CO_2(g)$	Calcite saturation index	Calculated alkalinity (calculated from pH and TIC)	Reported Alkalinity
		Min	Middle	Max		Litres/minute	Litres	mg/L			meq/l	meq/l
Units		mbgl	mbgl	mbgl								
AKEYO F.												
168	MSB-4	15.8	20.75	25.7	3		583		-2.21	0.16	3.51	
169	MSB-4	34.8	48.5	62.2	3		602		-2.66	0.32	2.98	
	MSB-4	15.8	20.75	25.7	3		583		-1.98	-0.05	3.70	
	MSB-4	26.5	30.2	33.9	3		1839		-2.84	0.60	3.16	
	MSB-4	34.8	48.5	62.2	3		602		-2.66	0.38	3.23	
	DH-15	63.0	67.75	72.5	3	2.5	3145.9	0.005	-3.75	-0.01	2.32	2.52
	DH-15	84.5	91	97.5	3	6	21738	0.01	-4.05	0.11	2.50	2.6
TOKI LIGNITE BEARING F. (LOWER)												
1	KNA-6 sed.	-			2				-4.59	0.17	1.84	
2	KNA-6 unconf.	-			2				-4.18	0.16	2.00	
2	KNA-6 unconf.	-			2				-4.42	0.18	2.02	
150	DH-12	157.5	160.79	164.1	2	0.25	690	0.03	-5.21	0.08	0.95	1.1
159	MIU-4	71.5	74.11	76.8	2	0.35	1913	0.01	-4.49	0.0099	1.77	1.76
164	MSB-2	79.0	104.75	130.5	2	7.9	34626.4	0.01	-4.63	0.2297	0.58	0.68
165	MSB-2	132.0	142.99	154.0	2	4	11083	0.01	-4.52	0.0195	0.38	0.45

Physico-chemical parameter measuring location: 1 = in-situ measurement; 2 = flow-through cell; 3 = laboratory measurement

Table A4-2 continued.

Index	Location	Depth			Physico-chemical parameter measuring location	Pumping rate	Total extracted water volume	DO	log f $CO_2(g)$	Calcite saturation index	Calculated alkalinity (calculated from pH and TIC)	Reported Alkalinity
		Min	Middle	Max		Litres/minute	Litres	mg/L			meq/l	meq/l
		mbgl	mbgl	mbgl								
3	KNA-6 gra.	-			2				-3.12	0.01	1.97	
3	KNA-6 gra.	-			2				-3.49	0.21	1.71	
170	DH-2	207.5	208.5	209.5	2				-3.74	0.0813	1.06	
171	DH-2	228.5	232.75	237.0	2				-3.94	0.1814	0.94	
172	DH-2	302.7	303.7	304.7	2				-4.44	-0.1763	0.35	
173	DH-2	305.6	306.55	307.6	2				-4.24	0.1044	0.64	
174	DH-2	309.7	310.7	311.7	2				-4.25	0.2317	0.65	
175	DH-2	313.0	314	315.0	2				-4.12	0.1506	0.65	
176	DH-2	320.9	324.65	328.4	2				-4.06	0.0151	0.63	
177	DH-2	347.8	348.8	349.8	2				-4.33	0.1367	0.50	
178	DH-2	365.5	366.5	367.5	2				-4.37	0.1327	0.47	
179	DH-2	439.5	443.75	448.0	2				-4.43	0.2146	0.44	
180	DH-2	451.2	455.45	459.7	2				-4.36	0.1905	0.41	
	DH-7	438.0	441.25	444.5	3				-4.29	0.23	Not calculated	0.73
	DH-7	479.0	482.25	485.5	3				-6.45	0.88	Not calculated	0.89
	DH-7	479.0	482.25	485.5	3				-5.69	0.67	Not calculated	0.83
108	DH-7	560.5	563.75	567.0	1	0.031	292		-5.39	0.94	3.63	1.51
	DH-7	560.5	563.75	567.0	3				-6.79	0.74	Not calculated	1.25

Table A4-2 continued.

Index	Location	Depth			Physico-chemical parameter measuring location	Pumping rate	Total extracted water volume	DO	log f CO_2(g)	Calcite saturation index	Calculated alkalinity (calculated from pH and TIC)	Reported Alkalinity
		Min	Middle	Max		Litres/minute	Litres	mg/L			meq/l	meq/l
		mbgl	mbgl	mbgl								
	DH-7	560.5	563.75	567.0	3				-6.35	0.51	Not calculated	0.83
	DH-7	598.0	601.25	604.5	3				-8.58	-0.02	Not calculated	1.49
	DH-7	598.0	601.25	604.5	3							1.26
	DH-7	660.0	663.25	666.5	3				-6.03	0.91	Not calculated	0.97
	DH-7	660.0	663.25	666.5	3							1.01
	DH-7	735.5	738.75	742.0	3							2.08
	DH-7	735.5	738.75	742.0	3							1.96
109	DH-7	833.5	836.75	840.0	1	0.039	228.1		-4.67	0.55	2.59	1.65
	DH-7	833.5	836.75	840.0	3				-7.51	0.43	Not calculated	1.48
110	DH-7	880.0	883.25	886.5	1	0.04	199.4		-4.40	0.68	3.21	1.79
	DH-7	880.0	883.25	886.5	3				-7.11	0.53	Not calculated	1.63
	DH-7	880.0	883.25	886.5	3				-8.38	-0.30	Not calculated	1.55
151	DH-12	171.8	225.99	280.2	2	160	677698	0.01	-4.82	0.2	0.70	0.679
155	DH-12	431.4	451.96	472.5	2	140	53405	0.02	-4.79	0.25	5.8	0.635
156	DH-12	388.9	409.29	429.7	2	42.3	133199	0.01	-4.73	0.18	0.34	0.373
157	DH-12	345.9	366.54	387.2	2	52	379857	0.02	-4.64	0.17	0.40	0.435
158	DH-12	279.4	312.04	344.7	2	48.5	128543	0.020	-4.86	0.24	0.41	0.523
160	MIU-4	82.3	99.37	116.5	2	4.4	19337.5	0	-4.27	0.21	1.71	1.54

Table A4-2 continued.

Index	Location	Depth			Physico-chemical parameter measuring location	Pumping rate	Total extracted water volume	DO	log f $CO_2(g)$	Calcite saturation index	Calculated alkalinity (calculated from pH and TIC)	Reported Alkalinity
		Min	Middle	Max		Litres/minute	Litres	mg/L			meq/l	meq/l
		mbgl	mbgl	mbgl								
161	MIU-4	272.8	273.62	274.5	2	4.5	40080.3	0.02	-4.57	0.30	1.54	1.44
162	MIU-4	505.8	533.09	560.4	2	10	28000	0	-4.34	0.21	1.47	1.4
163	MIU-4	653.4	668.84	684.3	2	4.5	19180	0	-4.30	0.32	1.62	1.55
166	MSB-2	171.5	173.49	175.5	2	1.2	11700.1	0.01	-4.25	0.01	0.48	0.56
167	MSB-4	95.5	97.25	99.0	2	5.5	2159.1	0.01	-4.18	0.18	0.84	0.77
	MIZ-1	113.1	114.67	116.3	2	44	46303.5	0	-4.57	0.16	0.94	1.27
	MIZ-1	215.0	220.34	225.7	2	30	101826	0	-4.45	0.06	0.88	0.68
Units		mabh	mabh	mabh		litres/minute	litres	mg/L				
TOKI GRANITE												
	MIZ-1	580.80	588.95	597.10	2		3133	0.0	-4.50	0.2019	0.58	0.56
	MIZ-1	649.00	687.48	725.96	2		19127	0.0	-4.50	0.2354	0.41	0.39
TOKI LIGNITE BEARING F. (LOWER)												
	DH-15	102.70	118.2	133.70	2		2522	0.00	-5.51	0.4607	1.56	1.74
	DH-15	152.10	184.27	216.43	2		61080	0.00	-4.78	0.1447	1.22	1.04
TOKI GRANITE												
	DH-15	233.55	236.78	240.00	2		35793	0.00	-4.60	0.1905	0.88	0.61

Table A4-2 continued.

Index	Location	Depth			Physico-chemical parameter measuring location	Pumping rate	Total extracted water volume	DO	log f CO_2(g)	Calcite saturation index	Calculated alkalinity (calculated from pH and TIC)	Reported Alkalinity
		Min	Middle	Max		Litres/minute	Litres	mg/L			meq/l	meq/l
		mbgl	mbgl	mbgl								
	DH-15	437.60	449.85	462.1	2		36601	0.00	-4.25	0.0756	0.58	0.57
	DH-15	575.50	587.75	600.00	2		82709	0.00	-4.04	-0.2792	0.32	0.36
	DH-15	765.00	773.25	781.5	2		10172	0.00	-4.64	0.04	0.20	0.19
	DH-15	937.00	945.25	953.50	2		77009	0.00	-3.93	0.179	0.36	0.32
	DH-15	987.00	995.25	1003.5	2		127839	0.00	-5.05	0.1932	0.21	0.16

Notes:

🟨	Calculated for this study by R. Metcalfe
🟦	From Arthur, R.C. 2003. Empirical constraints on theoretical models of the chemical evolution of groundwaters in the Tono area. Monitor Scientific Draft Final Report

Sample container: 1 = downhole sampling vessel that maintains in-situ conditions; 2 = polythene bottle used to collect samples at the surface

Sampling location: 1 = downhole (1000 m sampling device, MP system etc); 2 = Sampled at the surface during a hydraulic test

Physico-chemical parameter measuring location: 1 = in-situ measurement; 2 = flow-through cell; 3 = laboratory measurement

Table A4-3 Estimates of data quality.

Index	Location	Depth			pH (major cations, major anions, PA-relevant trace constituents)		Eh		Redox-sensitive trace elements		Inorganic carbon species	
		Min	Middle	Max	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)
Units		mbgl	mbgl	mbgl								
AKEYO F.												
168	MSB-4	15.8	20.75	25.7	0.52	0.24	0.01	0.00	0.01	0.00	0.52	0.24
169	MSB-4	34.8	48.5	62.2	0.20	-0.20	0.01	0.00				
	MSB-4	15.8	20.75	25.7	0.52	0.24						
	MSB-4	26.5	30.2	33.9	0.50	0.25						
	MSB-4	34.8	48.5	62.2	0.20	-0.20						
	DH-15	63.0	67.75	72.5	0.76	0.12						
	DH-15	84.5	91	97.5	0.48	0.26						
TOKI LIGNITE BEARING F. (LOWER)												
1	KNA-6 sed.	-			71.00	0.29						
2	KNA-6 unconf.	-			71.00	0.29	68	0.32	66	0.34	2.84	0.04
2	KNA-6 unconf.	-			71.00	0.29						
150	DH-12	157.5	160.79	164.1	0.54	0.23						
159	MIU-4	71.5	74.11	76.8	34.00	0.66						
164	MSB-2	79.0	104.75	130.5	0.20	-0.20						
165	MSB-2	132.0	142.99	154.0	0.20	0.4	0.01	0.00	0.01	0.00	0.27	0.25
TOKI GRANITE												
3	KNA-6 gra.	-			0.67	-0.67						
3	KNA-6 gra.	-			0.66	-0.66						

Table A4-3 continued.

Index	Location	Depth			pH (major cations, major anions, PA-relevant trace constituents)		Eh		Redox-sensitive trace elements		Inorganic carbon species	
		Min	Middle	Max	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)
Units		mbgl	mbgl	mbgl								
170	DH-2	207.5	208.5	209.5	0.02	0.50						
171	DH-2	228.5	232.75	237.0	1.00	1.00						
172	DH-2	302.7	303.7	304.7	1.00	1.00						
173	DH-2	305.6	306.55	307.6	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
174	DH-2	309.7	310.7	311.7	0.02	0.50						
175	DH-2	313.0	314	315.0	1.00	1.00						
176	DH-2	320.9	324.65	328.4	1.00	1.00						
177	DH-2	347.8	348.8	349.8	1.00	1.00						
178	DH-2	365.5	366.5	367.5	1.00	1.00						
179	DH-2	439.5	443.75	448.0	1.00	1.00						
180	DH-2	451.2	455.45	459.7	1.00	1.00						
	DH-7	438.0	441.25	444.5	0.02	0.50						
	DH-7	479.0	482.25	485.5	0.02	0.50						
	DH-7	479.0	482.25	485.5	0.02	0.50						
108	DH-7	560.5	563.75	567.0	0.02	0.50	0.02	0.50	0.02	0.50	0.02	0.50
	DH-7	560.5	563.75	567.0	0.02	0.50						
	DH-7	560.5	563.75	567.0	0.02	0.50						
	DH-7	598.0	601.25	604.5	0.02	0.50						
	DH-7	598.0	601.25	604.5	0.02	0.50						
	DH-7	660.0	663.25	666.5	0.02	0.50						

Table A4-3 continued.

Index	Location	Depth			pH (major cations, major anions, PA-relevant trace constituents)		Eh		Redox-sensitive trace elements		Inorganic carbon species	
		Min	Middle	Max	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)
Units		mbgl	mbgl	mbgl								
	DH-7	660.0	663.25	666.5	0.02	0.50						
	DH-7	735.5	738.75	742.0	0.02	0.50						
	DH-7	735.5	738.75	742.0	0.02	0.50						
109	DH-7	833.5	836.75	840.0	0.02	0.50						
	DH-7	833.5	836.75	840.0	0.02	0.50						
110	DH-7	880.0	883.25	886.5	0.02	0.50						
	DH-7	880.0	883.25	886.5	0.02	0.50						
	DH-7	880.0	883.25	886.5	0.02	0.50						
151	DH-12	171.8	225.99	280.2	0.16	-0.16	0.05	-0.05	0.10	-0.10	0.22	-0.22
155	DH-12	431.4	451.96	472.5	0.09	-0.09						
156	DH-12	388.9	409.29	429.7	0.16	-0.16						
157	DH-12	345.9	366.54	387.2	0.10	-0.10						
158	DH-12	279.4	312.04	344.7	0.09	-0.09						
160	MIU-4	82.3	99.37	116.5	0.11	-0.11						
161	MIU-4	272.8	273.62	274.5	0.46	0.27						
162	MIU-4	505.8	533.09	560.4	0.11	-0.11	0.01	0.00	0.01	0.00	0.16	-0.16
163	MIU-4	653.4	668.84	684.3	0.18	-0.18						
166	MSB-2	171.5	173.49	175.5	0.62	0.19	0.01	0.00	0.01	0.00	0.66	0.17
167	MSB-4	95.5	97.25	99.0	0.54	0.23						
	MIZ-1	113.1	114.67	116.3	0.48	0.26						

Table A4-3 continued.

Index	Location	Depth			pH (major cations, major anions, PA-relevant trace constituents)		Eh		Redox-sensitive trace elements		Inorganic carbon species	
		Min	Middle	Max	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)	For/Against	Uncertainty (+ve) or Conflict (-ve)
Units		mbgl	mbgl	mbgl								
	MIZ-1	215.0	220.34	225.7	0.10	-0.10	0.01	0.00	0.01	0.00	0.06	-0.06
TOKI GRANITE												
	MIZ-1	580.80	588.95	597.10	0.01	0.00						
	MIZ-1	649.00	687.48	725.96	0.01	0.00						
TOKI LIGNITE BEARING F. (LOWER)												
	DH-15	102.70	118.2	133.70	0.01	0.00						
	DH-15	152.10	184.27	216.43	0.24	-0.24						
TOKI GRANITE												
	DH-15	233.55	236.78	240.00	0.70	0.15						
	DH-15	437.60	449.85	462.1	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00
	DH-15	575.50	587.75	600.00	0.01	0.00						
	DH-15	765.00	773.25	781.5	0.01	0.00						
	DH-15	937.00	945.25	953.50	0.01	0.00						
	DH-15	987.00	995.25	1003.5	0.24	-0.24						

Note: To avoid division of zero or division by zero, when calculating the ratio For/Against, any evidence values of zero are converted to a minimum of 0.01. This approach results in a possible ratio between 0.01 and 100. This approach is consistent with the approach adopted for plotting the ratio plot.