

Critical review: data production

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Recommendations

- According to their Chief Inspector, the fundamental purpose of the AAIB (UK Air Accidents Investigation Branch) is:

"To improve aviation safety by determining the causes of air accidents and serious incidents and making safety recommendations intended to prevent recurrence"

...It is not to apportion blame or liability.

- To be successful, QA must operate in the same manner....

Background

- As the national programme moves closer to realisation, it is necessary to develop and support the standards and practices which will be expected by Japanese stakeholders
- Clearly, quality assurance programmes are among the first such tools required and here the current level is examined with a few actual examples
- Unlike Yui-san, I do not believe that all is OK and I want to ask you what we need to do to improve the situation

Example - analysis

- Anions: F⁻, Cl⁻, Br⁻, NO₃⁻, NO₂⁻, SO₄²⁻ (Table 6 attached to Notification No. 59 of the Ministry of the Environment, JIS K0102 35.3, 41.3, 43.1 and 43.2)
- Filter the reagent water through a filter (0.45µm pore size) used for Ion Chromatograph system. Measure the anions in the filtered water.
- Anions :PO₄³⁻, I⁻ (JIS K0102 46.1.1 and 35.3)
- Filter the reagent water through a filter (0.45µm pore size) used for Ion Chromatograph system. Measure the anions in the filtered water.
- Total-Fe Electrothermal Atomic Absorption Spectrometric (ETAAS) method (JIS K0101 58.4)

Analysis

- This is an example from the Mizunami URL QA system and it is excellent
- It goes on to describe the analytical procedures in detail and will be the model for the upcoming Horonobe system
- BUT.....

Analysis

		X	Y
Ti ⁴⁺	[mg/l]	-	-
Fe(III)	[mg/l]	0.02	0.03
Fe(II)	[mg/l]	<0.01	0.03
Total-Fe	[mg/l]	-	-
Al ³⁺	[mg/l]	<0.1	<0.1
F ⁻	[mg/l]	<0.1	<0.1
Cl ⁻	[mg/l]	2730	4180
Br ⁻	[mg/l]	10	19
NO ₃ ⁻	[mg/l]	<0.1	<0.1
NO ₂ ⁻	[mg/l]	<0.1	<0.1
SO ₄ ²⁻	[mg/l]	8.7	2.4
S ²⁻	[mg/l]	-	-
Total-B	[mg/l]	-	0.6
Total-Be	[mg/l]	-	-
Total-Cr	[mg/l]	-	-
Total-Co	[mg/l]	-	-
Total-Ni	[mg/l]	-	-
HCO ₃ ⁻	[mg/l]	1430	2120
CO ₃ ²⁻	[mg/l]	-	-

Analysis

➤ Element/species	Detection limit	Uncertainty
Ti ⁴⁺	0.01mg/L	±5% of Measured value
Fe(III)	0.01mg/L	±5% of Measured value
Fe(II)	0.01mg/L	±5% of Measured value
Total-Fe	0.01mg/L	±5% of Measured value
Al ³⁺	0.01mg/L	±5% of Measured value
F ⁻	0.1mg/L	±5% of Measured value
Cl ⁻	0.1mg/L	±5% of Measured value
Br ⁻	0.1mg/L	±5% of Measured value
NO ₃ ⁻	0.1mg/L	±5% of Measured value
NO ₂ ⁻	0.1mg/L	±5% of Measured value
SO ₄ ²⁻	0.1mg/L	±5% of Measured value
S ²⁻	0.1mg/L	±5% of Measured value
Total-B	0.02mg/L	±5% of Measured value
Total-Be	0.05mg/L	±5% of Measured value
Total-Cr	0.05mg/L	±5% of Measured value
Total-Co	0.05mg/L	±5% of Measured value
Total-Ni	0.05mg/L	±5% of Measured value
HCO ₃ ⁻	0.1mg/L	±5% of Measured value
CO ₃ ²⁻	0.1mg/L	±5% of Measured value

Analysis

- This is an example from Japan, but the same thing has happened in Europe
- SKB's hydrochemistry database (SICADA) contains no uncertainties
- Constant lobbying over the last 2 years means this will be changed shortly.....but uncertainty values on laboratory data follow the same pattern

Data reporting - uncertainties

- In base publications **all** assessment of errors and uncertainties should be **explicitly** documented
- Overview or synthesis publication may summarise such analysis, but should still report
 - Total errors on measured data
 - Results of replicate analysis
 - Results of measurements of standards
- Errors should be shown in all data presentations - including tables **and figures**
 - Precision indicates the number of significant figures that should be presented (e.g. beware of 1.23456 +/- 10!)
- ➔ **Demonstration of a clear understanding of uncertainties is critical to establishing credibility in the field of radwaste disposal**

Evaluation of the literature (1)

- Despite all the discussion above, the peer-reviewed literature is full of examples where either errors are not presented, are insufficiently documented or are wrongly interpreted
- As a general indicator:
 - No reported errors in article - this is not worth wasting time on
 - This also is indicative of the poor quality of peer-review of the journal/report series and hence all material from the same source should be considered suspect (e.g. ARAP series)
 - Only 1 σ counting errors reported - **treat with great caution**; trends in data may be useful, but absolute values must be considered suspect

Evaluation of the literature (2)

- As a general indicator (cont):
 - Errors discussed but not shown on figures (or treated incorrectly - eg data to unreasonable numbers of significant figures, **incorrect error bars on log transformed data**, ...) - **treat with great caution**; data may be useful, but interpretation must be considered suspect
 - Comprehensive treatment of errors - **evidence of competent measurement**; does not, however, provide any guarantee on quality of subsequent data interpretation!
- ➔ **Treat the literature with great caution; assess critically even if from “established” authors, journals or institutes! This is of great importance for the PIA of any volunteer site**

Evaluation of the literature (3)

Table 3 Distribution coefficients of the radionuclides in both adsorption (K_d^{ads}) and desorption (K_d^{des}) processes.

	Distribution coefficient (cm^3/g)			
	^{85}Sr	^{237}Np	^{238}Pu	^{241}Am
K_d^{ads}	130	71	1200	>10000
K_d^{ads} (after 450 nm filtration)	130	78	1400	>10000
K_d^{des}	160	110	1200	>10000

Total uncertainty (1)

- An error or uncertainty should be associated with **every** measurement made: the total **random** error can then be calculated by propagating errors over the entire calculation used to produce the data to be used: for example

$$C = ((M - B) * E / W) \exp(\lambda t)$$

C - activity concentration at time=0 (Bq / kg)

M - measured activity at time=t (cps)

B - background (cps)

E - efficiency (Bq / cps)

W - weight (kg)

λ - decay constant (/day)

t - time between sampling and counting (days)

- Error propagation may be simplified if some errors are sufficiently small compared to the others that they can be ignored, but total error is readily determined by simple spreadsheet calculations

Total uncertainty (2)

- The random error on the measurement does not include all the uncertainties associated with the process of sampling, handling and processing for counting - these can only be determined by measuring replicate samples to determine the overall precision
- **NB it is common for environmental measurements to have calculated errors on single measurements in the % range, whereas replicate samples may scatter by factors of 2-3 or more (indeed order of magnitude variations are not unknown!!!).**
- It is usually assumed that measured data follow a normal distribution - hence this is derived from replicate measurements using:

s - standard deviation

N - number of replicates

x_i - individual measurements

\bar{x} - mean of the measurements

$$s = \sqrt{\frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2},$$

Total uncertainty (3)

- **Systematic errors are assessed by either running recognised standard samples (if available) or artificially preparing appropriate such materials**
 - **These materials must be subject to as much of the sampling and preparation process as possible - but this may be inherently limited (e.g. for deep groundwaters or ocean sediments)**
- **There will always be residual uncertainties - the challenge is to minimise them....**

So what now?

- **Basically, we need to look at everything in a cautious manner and assume the worse**
- **What can we do with the existing data?**
 - **Retro-QA**
- **What shall we do with new data?**
 - **ISO 9001, 14001 etc**

Retro-QA

- Ian noted that 'Retro-QA' is not easy, but it is not impossible
- Work currently ongoing at Horonobe to QA existing hydrochemistry data
- To save re-inventing the wheel, we have turned to SKB's ongoing site characterisation (at Forsmark and Laxemar)
- Here, some very stringent data requirements (from the site assessment group and the regulators) led to the development of a system of ranking the analytical data based on a suite of criteria
- System also used by Posiva (NB they dump data....)

QA formalisation

- Categories 1-3 primarily meet the requirements of hydrochemical (but also hydrogeological) modelling, while categories 4-5 primarily meet hydrogeological requirements (but may also be of use for more qualitative hydrochemical modelling with caution)
- A colour code has been defined to make sample identification easier when data are presented in spreadsheets or in scatter plots:
 - Category 1 is orange
 - Category 2 is yellow
 - Category 3 is green
 - Category 4 is grey
 - Category 5 is black

QA formalisation

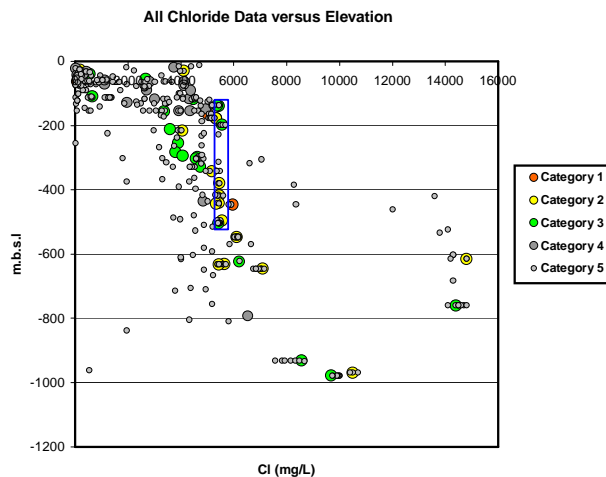
Cored Boreholes	Category				
<i>Aspects/Conditions</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>
Drilling water ($\leq 1\%$)	x	x	x	x	x
Drilling water ($\leq 5\%$)		x	x	x	x
Drilling water ($\leq 10\%$)			x	x	x
Drilling water ($> 10\%$)				x	x
Time series (adequate)	x	x	x	x	x
Time series (inadequate)			x	x	x
Time series (absent)				x	x
Suitable section length	x	x	x	x	x
Sampling during drilling				x	x
Sampling during hydraulic testing			x	x	x
Tube sampling					x
Charge balance $\pm 5\%$ ($\pm 10\%$ for < 50 mg/L Cl)	x	x	x	x	x
Major ions (complete)	x	x	x	x	x
Major ions (incomplete)			x	x	x
Environmental isotopes (complete)	x	x	x	x	x
Environmental isotopes (incomplete)			x	x	x
Hydraulic effects (short-circuiting)	x	x	x	x	x

QA – porewaters

Porewaters	Category				
<i>Aspects/conditions</i>	<i>1</i>	<i>2</i>	<i>3</i>	<i>4</i>	<i>5</i>
Drilling fluid ($\leq 10\%$)	X	X	X	X	X
Drilling fluid ($\leq 50\%$)		X	X	X	X
Drilling fluid ($> 50\%$)				X	X
Oxidation/CO ₂ reaction			X	X	X
QAd sampling methodology	X	X	X	X	X
QAd analytical data, including uncertainties	X	X	X	X	X
Chlorinity	X	X	X	X	X
δD	X	X	X	X	X
$\delta^{18}O$	X	X	X	X	X
3H		X	X	X	X
Major elements			X	X	X
pH			X	X	X
Alkalinity			X	X	X
Immediately adjacent groundwater analysis available		X	X	X	X

QA formalisation

Here, all five categories are plotted for Cl vs depth. This shows that the general trends and important outliers indicated by all data are strengthened and constrained by the higher category samples (1-3). The lower quality category 4 & 5 samples show the greatest scatter, but even so many follow the major trends.



Retro-QA

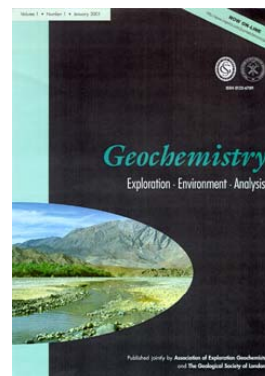
- Assessing groundwater quality and assigning a QA **category of suitability** requires an evaluation of all the available hydrochemical data with reference to known hydraulic conditions in:
 - the borehole
 - the fracture zone sections being sampled
 - the surrounding host bedrock (rock matrix)
- the reliability of these data is judged on prevailing hydraulic and geologic conditions during drilling and subsequent monitoring/sampling
- without the integration of hydrochemistry, geology, hydrogeology and **borehole activities** there is a great danger that data (quality) can be misrepresented

Retro-QA

- to date, the Horonobe QA approach has only been used on recently produced data where the background information is either complete enough and/or the `company memory` still exists
- nevertheless, the approach is also valid for older data – and indeed would be a *necessity* when evaluating existing data at a volunteer site
- further, all new data for Horonobe will be QAd in this formal manner and the database will be frozen
 - *for new boreholes, this is required to place the new data in context in the site conceptual model*
 - *for existing boreholes, this is required to provide higher category data for interpretation and modelling purposes*

Retro-QA

- This work will be presented in detail (in Japanese) at the Annual Meeting of the Atomic Energy Society of Japan (Tokyo Institute of Technology, 23rd – 25th March 2009)
- Will also be presented (in English) at the Borehole Workshop on Friday
- And is described in a paper which will be submitted to the journal **Geochemistry: Exploration, Environment, Analysis** very shortly



ISO

- Do we need ISO?
- How would it help?
 - It sets out a series of steps which need to be taken
 - BUT it does not check if the processes or approaches are fundamentally correct
 - Nor does it check if our tools are fit-for-purpose
 - Nor does it say when we need to act or how to set priorities
- What do we need? Group exercise.....

Yes we can.....

- Stakeholders need to know that QA standards in the national programme are the best in the world
- and they will be
- because we can!

Yes we must.....

ASN criticises methodology at EdF monitoring labs

World Nuclear News 13 January 2009

- **The French Nuclear Safety Authority (Autorité De Sûreté Nucléaire, ASN) has decided to refuse or suspend the accreditation of laboratories run by Electricité de France (EdF) for monitoring radioactivity in the environment around its plants.**

As of 1 January, the ASN has made it a requirement that laboratories measuring radioactivity in the environment must be subjected to a procedure of accreditation. It earlier set up an accreditation committee responsible for issuing an opinion on the technical quality of applications submitted by such laboratories.