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A Quality Assurance Procedure for Aquifer Property and Chemistry Data in the Northern Ireland Groundwater Data Repository

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Quality Assurance Procedures for Aquifer Property and Chemistry Data in the Northern Ireland Groundwater Data Repository

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Summary

This report describes the quality assurance (QA) procedures used to ensure the reliability of hydrogeological – aquifer properties and groundwater chemistry – data added to the Northern Ireland Groundwater Data Repository (NIGDR).

Section 1 introduces the NIGDR and the need for QA procedures. Section 2 describes the QA procedures applied to aquifer properties data and Section 3 describes the procedures applied to groundwater chemistry data.

1 Introduction

The Northern Ireland Groundwater Data Repository (NIGDR) was created in 2017 (O'Dochartaigh and Wilson, 2021). It is a central database of aquifer property and chemistry data, created, managed and maintained by the Geological Survey of Northern Ireland (GSNI) as a safe long-term storage solution for the many disparate sources of hydrogeological data that could otherwise be lost or forgotten. This database is an asset of national importance, which can support important research and decisions about how the groundwater resources of Northern Ireland can be used and managed sustainably.

The hydrogeological information held in the NIGDR includes data on physical aquifer properties and groundwater chemistry. These data come from various sources, some of which are more reliable than others. The reliability of hydrogeological data depends on where the data comes from, and how it was collected and analysed. To ensure confidence in the data its reliability, or quality, must be assessed and categorised in a transparent and consistent way, which needs information on the characteristics of data collection and analysis.

Before being added to the NIGDR, all the data were subject to consistent Quality Assurance (QA) procedures, in order to provide confidence in the data for future use. This document describes the QA procedures used. Different procedures were used for aquifer properties (Section 2) and groundwater chemistry (Section 3) data.

2 Aquifer Property Data Quality Assessment Procedures

2.1 WHAT ARE AQUIFER PROPERTIES DATA

Aquifer properties data are quantitative data describing the physical properties of aquifers. Key aquifer properties are transmissivity, permeability, porosity, storage capacity (including storativity and specific yield). Additional very useful quantitative data, particularly if there are few or no other data, are specific capacity and borehole yield, both of which show a significant correlation with transmissivity (Graham et al. 2009). Rest water level data can also be considered a physical aquifer property, although it is also (and more strongly) related to transient climatic and weather conditions.

These data are derived from various aquifer tests. The most important tests that provide aquifer properties data are test pumping of boreholes, and laboratory analysis of aquifer materials (eg for aquifer matrix permeability and porosity).

The reliability of aquifer properties data depends on the suitability and application of test procedures and of post-test analysis methods, and on post-analysis data management. (Allen et al., 1997)

2.2 OVERVIEW OF QUALITY ASSESSMENT PROCEDURE FOR AQUIFER PROPERTIES DATA

Quality assessment and quality control of water sampling and analysis results is known to be a vital component in any sampling, analysis and report system for testing the quality of environmental waters (British Standards Institution, 2014). The key aim of this QA procedure is to assign a data quality category to each data value. This category represents an objective, consistent, transparent assessment of the reliability of each data value, based on information on how the value was collected and analysed. For aquifer properties in the NIGDR, each data value was assigned a data quality category of A, B or C, to represent High, Moderate or Low reliability, or data quality.

In cases where there is more than one parameter value for a single groundwater source (in most cases a borehole or spring), a second stage of the QA procedure is to derive a single preferred value from the multiple individual parameter values, and to assign the preferred value its own data quality category. This second stage is needed in many cases. In the case of pumping test data, it may be because data from more than one pumping test on a single borehole are available, or because more than one calculation method was used to analyse data from a single pumping test. In the case of core analysis data, there are usually a number of core samples from different borehole depths and many different porosity values for a single borehole. In the case of aquifer properties derived from borehole test pumping – such as transmissivity - storing more than one value for a single borehole could skew later data interpretation. However, in other cases, variations for a single borehole may be of critical interest in hydrogeological studies – such as variations in matrix porosity and permeability with depth. In this case, if there are multiple values for a single borehole it may be important to keep all of them as well as deriving a single preferred value.

In summary, the quality assessment (QA) procedure for aquifer properties data added to the NIGDR involves

- Assigning a data quality category for each data value based on an assessment of:
 - the type, details and rigorousness of the tests used to measure aquifer properties (eg test pumping, or laboratory analysis of porosity)
 - the method, details and rigorousness of analysis methods applied to raw test data (e.g. Jacob's approximation for transmissivity applied to test pumping data, or numerical pump test analysis models applied to test pumping data)
- Assigning a preferred aquifer properties value if more than one value is available for a single groundwater source
- Being transparent about the QA assessment, including following the QA procedures described in this document, and adding any relevant additional information to the NIGDR (in Notes field) that may aid transparency.

2.3 ASSIGNING A DATA QUALITY CATEGORY TO EACH AQUIFER PROPERTY VALUE

Assigning a data quality category to each aquifer property value is done following a series of consistent rules. These rules are described below for:

- data from pumping tests, or other pumping data¹ (Table 1)
- data from spring flow monitoring, either spot or continuous gauging using normal methods such as velocity area or dilution gauging
- data from laboratory tests (Table 2); and
- Other data – in the case of the NIGDR this is rest water level data (Table 3)

There are also supplementary guidelines (Section 2.1.1), which essentially state that in the absence of information, or in any case where there is cause for doubt as to the quality of the data, a lower data quality is assigned to an individual value.

Data from pumping tests, other pumping data and spring flow data			
	A (High)	B (Moderate)	C (Low)
Transmissivity (T [m²/day])	<ul style="list-style-type: none"> • CR test ≥ 1 day with constant rate throughout and OBH and PBH data, or • PBH data only and drawdown or recovery data or both 	<ul style="list-style-type: none"> • CR test < 1 day, or • CR test ≥ 1 day with variable rate or step test of any length and drawdown or recovery data or both 	<ul style="list-style-type: none"> • Slug test, or • Test length or type not known or test data reveal poor test (eg varying pumping rates/not starting at RWL)
Storativity/Storage coefficient (S [-])	as T	as T	as T
Specific yield (Sy [-])	as T	<ul style="list-style-type: none"> • as T 	as T
Specific capacity (Sc or Q/s [m³/day/m])	<ul style="list-style-type: none"> • Reliable pumping test ≥ 1 day, or • NOY ≥ 2 years and normal stable drawdown 	<ul style="list-style-type: none"> • Reliable pumping test < 1 day, or • Of unknown length, or • NOY < 2 years and normal stable drawdown 	Unknown data source
Yield (Q [m³/day])	<ul style="list-style-type: none"> • Pumping test ≥ 1 day and drawdown $< 20\%$ of borehole depth, or • NOY ≥ 2 years and normal stable drawdown. or • High resolution ($>$ hourly) continuous spring flow data ≥ 1 year 	<ul style="list-style-type: none"> • Pumping test ≥ 1 day and drawdown $> 20\%$ of borehole depth, or • Pumping test < 1 day or of unknown length, or • NOY < 2 years and normal stable drawdown, or • Other spring flow data 1-5 years 	<ul style="list-style-type: none"> • Non-pumping test data, or • Unknown data source, or • Other spring flow data < 1 year

¹ Normal Operating Yield (NOY) is the normal yield of water pumped from a borehole under normal operation. This can provide a minimum estimate of a borehole yield, and when normal stable drawdown is known, specific capacity can be estimated also.

Table 1 Aquifer property data quality categories for data from pumping tests, and other pumping data and spring flow data

(Note: CR = constant rate; OBH = Observation borehole; PBH = Pumping borehole; NOY = Normal operating yield)

Data from laboratory tests			
	A (good or very good)	B (average or moderate)	C (poor)
Porosity (Φ [%])	Known lab with known quality standards	Known lab with unknown quality standards	Unknown data source
Lab intrinsic permeability (k [m/d])	Known lab with known quality standards	Known lab with unknown quality standards	Unknown data source

Table 2 Aquifer property data quality categories for data from laboratory tests

Other data			
	A (good or very good)	B (average or moderate)	C (poor)
Rest water level (mbgl)	From a high quality pumping test or known reliable value from other source (e.g. monitoring ²)	Other pumping test data	Other quoted source (e.g. drillers' log) or unknown data source

Table 3 Aquifer property data quality category for rest water level data

2.3.1 Supplementary guidelines

It is common for aquifer properties data to be available with little or no metadata or supporting information on how or from where the data was derived. These guidelines supplement the rules in Table 1, Table 2 and Table 3 in cases where such supporting information is lacking.

The guidelines essentially state that in the absence of information, or in any case where there is cause for doubt as to the quality of the data, a lower data quality is assigned to an individual value.

For example, this may be where it is not clear whether available data were obtained from a pumping test or not, or, how long a pumping test was run for. By further example, in the latter case, in the absence of relevant information on the length of a pumping test, the test is assumed to have lasted for the shortest possible period (less than one day), and therefore is assigned data quality 'B' rather than 'A' (Table 1).

Supplementary guidelines:

- Where a value for a parameter is given in the absence of any other information on a borehole (e.g. pumping frequency, rest water level, pumped water level,

² Water level monitoring can include spot measurements using some form of dipper or continuous monitoring using some form of logging device such as a pressure transducer.

yield, mention of pumping test), it is treated as being of poor quality (quality category 'C').

- Where there is a value for both rest water level and pumped water level, a pumping test is assumed to have been carried out (quality category 'B').
- Where there is a value for rest water level and yield, a pumping test is assumed to have been carried (quality category 'B').
- Where the yield is given, along with an operational frequency of 24 hours per day and the absence of a rest water level reading, the value is assumed to be the normal operating yield for the borehole, in the absence of other information (quality category 'A' or 'B').
- If information provided shows internal inconsistencies or other clear errors, the data is normally treated as being poor (quality category 'C'), unless the errors do not put the reliability of the relevant parameters in doubt (e.g. data can be verified from another source; error is trivial, such as a spelling mistake).
- Where seasonal variability is quantitatively described, rest water levels are assumed to have been obtained through reliable monitoring of the borehole (quality category 'A').
- Where there is information to suggest that the value of a parameter has changed since the value provided (e.g. 'has suffered from declining yields'), values of rest water level and yield are deemed to be of poor quality (quality category 'C').
- Where a step test has employed a large number of discharge rates, interpreter discretion has been used to determine which yield values lie significantly below the maximum sustainable yield of the borehole. These values have not been included in calculations of preferred yield.

2.4 DERIVING A PREFERRED VALUE WHERE THERE IS MORE THAN ONE VALUE PER GROUNDWATER SOURCE

If there is more than one aquifer property value for a single groundwater source (usually a borehole), the rules below describe how a single preferred value (PV) is derived for each individual source.

2.4.1 Preferred aquifer property value where there is more than one value per pumping test

2.4.1.1 TRANSMISSIVITY

- General rule for constant rate (CR) tests: if observation borehole data are available, they are given priority, followed by abstraction borehole data. Multiple values from observation boreholes (OBHs) are averaged geometrically (since they may represent different areas of the aquifer). Multiple values from pumping boreholes (PBHs) are averaged arithmetically (since they represent different estimates of T at the same site).
 -
- For CR tests with 1 OBH:
 - Do not use T value from pumping borehole (PBH) data
 - From the OBH, if the analyst indicated one T value as best (eg according to analysis method assumptions best fitting the aquifer conditions), this is taken.
 - If there is no indicated or clear best value, take the arithmetic mean of all T values for the OBH
 - Assign the PV T value to the PBH

- For CR tests with >1 OBH:
 - Do not use T value from PBH data
 - For each OBH, if the analyst indicated one T value as best (eg according to analysis method assumptions best fitting the aquifer conditions), this is taken.
 - If there is no indicated or clear best value for each OBH, take the arithmetic mean of all T values for the OBH
 - Calculate the geometric mean of the interim PV's from each OBH
 - Assign the final PV T value to the PBH
-
- For CR tests with no OBHs:
 - If the analyst indicated one T value as best (eg according to analysis method assumptions best fitting the aquifer conditions), this is taken.
 - If there is no indicated or clear best value, take the arithmetic mean of all T values for the PBH
-
- If step-test data or data of unknown type only are available, they are averaged arithmetically.

2.4.1.2 STORAGE COEFFICIENT

- If the analyst indicated one as the 'best value', this is taken as the PV.
- If there is no indicated best value, but the hydrogeologist entering the data identifies one as the best value based on available data quality assessments, this is taken.
- Where no one value is identified as the best value, all the available data are averaged geometrically.

2.4.1.3 SPECIFIC CAPACITY

- If the analyst indicated one as the 'best value', this is taken as the PV.
- If there is no indicated best value, but the hydrogeologist entering the data identifies one as the best value based on available data quality assessments, this is taken.
- Where no one value is identified as the best value, use these rules:
 - For constant rate tests, data from tests ≥ 24 hours are given priority, followed by data from tests < 24 hours.
 - If step test data or data of unknown type only are available, they are averaged arithmetically

2.4.1.4 REST WATER LEVEL (RWL)

- There is not single preferred value for rest water level, as it is time dependent.
- Where there is >1 value, the minimum and maximum measured value are entered.
- Where there are long term (>1 year) data, an assessment of the normal annual range should be made and entered. Where relevant, a maximum and minimum annual range should also be entered.

2.4.1.5 YIELD

- If one value has a higher data quality category than the others, take this as the PV
- If all the values for a single site have the same data quality category, take the arithmetic mean of them all as the PV

2.4.2 Preferred aquifer property value where there is more than one value per groundwater source (e.g. >1 pumping test per source)

- If there is >1 value per test, first select the preferred value for each test, as above.

Then:

- If one test has a higher data quality rating than the others, it is selected.
- If >1 test has the highest quality rating, take the arithmetic average of the preferred test values.

3 Aquifer Chemistry Data Quality Assessment Procedures

3.1 WHAT ARE GROUNDWATER CHEMISTRY DATA

Groundwater chemistry data are quantitative data describing the chemistry of groundwater. Groundwater chemistry parameters may include inorganic major, minor and trace ions; conductivity and pH; dissolved gases such as oxygen, carbon dioxide, radon, methane or the industrial gases CFC and SF6 which can indicate residence time; and stable isotopes such as deuterium and oxygen 18.

Groundwater chemistry data are derived from various field and or laboratory tests and analyses. The reliability of groundwater chemistry data depends on sample collection procedures, field and laboratory analysis methods and procedures, and post-analysis data management.

3.2 OVERVIEW OF QUALITY ASSESSMENT PROCEDURE FOR GROUNDWATER CHEMISTRY DATA

The key aim of the QA procedure is to assign a data quality category to each data value. This category represents an objective, consistent, transparent assessment of the reliability of each data value, based on information on how the value was collected and analysed. One of five data quality categories has been assigned to groundwater chemistry data in the NIGDR: A, B, C, D, and R; plus an optional sixth qualifier category Z. These categories are described in detail in Table 5.

In summary, the QA procedure for groundwater chemistry data added to the NIGDR involves:

- Assigning a data quality category for each data value based on an assessment of:
 - the procedures used for groundwater sampling
 - the quality of analytical data derived from laboratory tests, in two ways:
 1. By assessing the procedures and competence of the analytical laboratory carrying out the tests, and
 2. By calculating the ionic balance of the analysed major ions.
- Being transparent about the QA assessment, including following the QA procedures described in this document, and adding any relevant additional information to the NIGDR (in Notes field) that may aid transparency.

3.3 OVERVIEW OF DATA QUALITY ASSESSMENT PROCEDURE FOR GROUNDWATER CHEMISTRY DATA

Assigning a data quality category to each groundwater chemistry analysis (and to each chemistry value within that analysis) is done by following the series of consistent rules described in Table 5.

Data Quality code	Groundwater chemistry data criteria	Outcome for NIGDR
A	<p>Sampled by GSNI or BGS or other known relevant agency using known, documented and consistent sampling and analysis procedures.</p> <p>Analytical laboratory known.</p> <p>Analysis includes all major, minor and trace ions.</p> <p>Ionic balance within +/- 5%.</p>	Retain
B	<p>Sampled by GSNI or BGS or other known relevant agency using known, documented and consistent sampling and analysis procedures.</p> <p>Analytical laboratory known.</p> <p>Analysis includes all major, minor and trace ions.</p> <p>Ionic balance between +/- 5-10%.</p> <p>However, if ionic balance > +/- 10%, individually check the analysis and if there's a sensible reason for the imbalance (e.g. very low bicarbonate), class as B.</p>	Retain
C	<p>Sampled by any other agency, known or unknown.</p> <p>Sampling procedure not necessarily known.</p> <p>Not clear at which laboratory samples were analysed.</p> <p>Analysis generally limited to major and a few minor ions, but always enough to do an ionic balance</p> <p>Most trace ions not analysed for.</p> <p>Ionic balance within +/- 10%.</p> <p>However, if ionic balance > +/- 10%, individually check the analysis: if there's a sensible reason for the imbalance (e.g. very low bicarbonate), class as C.</p>	Retain
D	<p>Very incomplete analysis – often only a few parameters, not enough to do an ionic balance.</p>	Not added to NIGDR
R	<p>Duplicate analysis for the same groundwater sample, eg using mass spectrometry (MS) or optical emission spectrometry (OES)</p>	<p>Selected duplicate retained; rejected duplicate not added to NIGDR.</p> <p>See Section 3.4 for rules for selecting which duplicate to retain.</p>

Z plus data quality code according to rules above (A, B, C, D etc.) (e.g. ZA, ZB, ZC, ZD)	Analysis indicates possible point pollution	The code Z flags a case of possible groundwater pollution but also includes the data quality code according to general rules for analytical quality
----------------------------------------------------------------------------------------------------------------	---------------------------------------------	-----------------------------------------------------------------------------------------------------------------------------------------------------

Table 4 Data quality categories for groundwater chemistry analysis

3.4 DATA STANDARDISATION PROCEDURE

All the chemistry data to be added to the NIGDR is subject to the following standardisation procedures.

1. Standardise units:
 - a) Use mg/l for major ions
 - b) Use µg/l for minor/trace ions
2. Duplicate analyses for the same water sample (data quality category R in Table 4) (ie >1 analysis for individual ions from different analytical techniques): follow these rules:
 - a. Only one analysis is retained for each ion.
 - b. As a general rule, the retained analysis should be the one with the lowest analytical detection limit.
 - c. If there is no significant difference in detection limits, the value to be retained for individual ions in the NIGDR should be selected based on the rules in Table 5. These rules were originally developed for the Baseline Scotland groundwater chemistry dataset (MacDonald et al., 2017).

Parameter	Notes
DOC & NPOC	Were all samples filtered? If not, would be lumping together TOC and DOC
Al	Choose MS over OES, but can use OES if necessary.
As	Use MS only, not OES
B	Use MS only, not OES
Ba	Use MS by preference, but where no MS value, use OES value
Be	Use MS only. Don't use OES even where no MS data.
Br	Use colorimetry by preference over IC, but where no colorimetry value use IC value.
Cd	Use MS only, not OES.

Co	Use MS only, not OES.
Cr	Use MS only, not OES.
Cu	Use MS only, not OES.
Fe	Use MS by preference, but where no MS value, use OES value
La	Use MS only, not OES.
Li	Use MS only, not OES.
Mn	Use MS by preference, but where no MS value, use OES value
Mo	Use MS only, not OES.
Ni	Use MS only, not OES.
P	Use MS only, not OES.
Pb	Use MS only, not OES.
Sc	Use MS only, not OES
Se	Use MS only, not OES
Sr	Use MS by preference, but where no MS value, use OES value
U	Use MS only, not OES
V	Use MS only, not OES
Y	Use MS only, not OES

Zn	Use MS by preference, but where no MS value, use OES value, unless DL for OES is very high.
Zr	Use MS only, not OES

Table 5 Rules for selecting which analysis value to retain, based on Baseline Scotland.

(MacDonald et al., 2017). (DL=detection limit; MS=mass spectrometry; OES=optical emission spectrometry; IC=ion chromatography)

Glossary

Borehole A shaft drilled in to the ground from which groundwater can be abstraction or measured

Constant Rate A pumping test performed with a constant pumping rate

Detection Limit The minimum concentration of a parameter that can be identified.

Observation Borehole A borehole, located some distance away from a pumping borehole, whose change in water level is recorded during and after a pumping test

Lab intrinsic permeability A laboratory measurement of the relative ease with which a porous medium can transmit a fluid under a potential gradient. It is the property of the medium only and is independent of the fluid. Commonly, but imprecisely, taken to be synonymous with the term Hydraulic Conductivity which implies the fluid is water.

Porosity The ratio of the volume of the interstices to the total volume of rock or superficial deposit expressed as a fraction. Effective porosity includes only the interconnected pore spaces available for groundwater transmission; measurements of porosity in the laboratory usually exclude any void spaces caused by cracks or joints (secondary porosity).

Pumping Borehole A borehole, which has water pumped out of it for the purposes of water supply or performing a pumping test

Pumping Test A field testing procedure to quantify aquifer properties at a site involving pumping water out of (or less commonly injecting water into) an aquifer and measuring the effect on water levels in that aquifer and sometimes in adjacent strata. There are several different procedures employed depending on the physical properties to be quantified. A constant-rate pumping test is conducted at a steady rate of discharge or injection; a step-test increases the discharge in stages to a maximum value; a bailing test is conducted during the drilling process, using the bailer drilling tool as a water withdrawal method. *Jargon term*
Explanation for the uninitiated professional, layman or customer. You can copy and paste this text for any further entries.

Rest Water Level The standing water level in a borehole or well when it is not being pumped.

Storativity The volume of water an aquifer releases from or takes into storage per unit surface area of the aquifer per unit change in head.

Specific Yield The amount of water in storage released from a column of aquifer of unit cross sectional area under unit decline of head. Expressed as a dimensionless proportion of the saturated mass of that aquifer unit. Effectively synonymous with Storage, in an unconfined aquifer. Equivalent to Effective Porosity.

Specific Capacity The rate of discharge of water pumped from a borehole divided by the resulting drawdown of the rest water level in the borehole.

Step Test A pumping test in which the pumping rate is increased in stages after the water level has stabilised at the current pumping rate

Yield The volume of water pumped or discharged from a borehole, well or spring.

Normal Operating Yield The volume of water pumped or discharged from a borehole, well or spring during normal operation as a water supply production point.

Transmissivity The integral of the hydraulic conductivity of an aquifer over its saturated thickness. It relates to the ability of an aquifer to transmit water through its entire thickness.

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British Geological Survey holds most of the references listed below, and copies may be obtained via the library service subject to copyright legislation (contact libuser@bgs.ac.uk for details). The library catalogue is available at: <https://envirolib.apps.nerc.ac.uk/olibcgi>.

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